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***** Welcome to STN International *****

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 AUG 10 Time limit for inactive STN sessions doubles to 40 minutes
NEWS 3 AUG 18 COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS 4 AUG 24 ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS 5 AUG 24 CA/Caplus enhanced with legal status information for U.S. patents
NEWS 6 SEP 09 50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS 7 SEP 11 WEIDS, WEINDEX, and WEIX now include Japanese FTERM thesaurus
NEWS 8 OCT 21 Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS 9 OCT 21 Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS 10 NOV 23 Addition of SCAN format to selected STN databases
NEWS 11 NOV 23 Annual Reload of IFI Databases
NEWS 12 DEC 01 FFFULL Content and Search Enhancements
NEWS 13 DEC 01 DEXENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets
NEWS 14 DEC 02 Derwent World Patent Index: Japanese FI-TERM thesaurus added
NEWS 15 DEC 02 PCTGEN enhanced with patent family and legal status display data from INPADOCDB
NEWS 16 DEC 02 USGENE: Enhanced coverage of bibliographic and sequence information

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V9.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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***** STN Columbus *****

FILE 'HOME' ENTERED AT 09:21:19 ON 18 DEC 2009

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Uploading C:\Program Files\STNEXP\Queries\10591950-claim 1-v 1.str



chain nodes :
1 2 3 4 5 6 13 14
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 2-3 3-4 4-5 5-6 6-7 10-13 13-14
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact bonds :
1-2 2-3 3-4 4-5 5-6 6-7 10-13 13-14
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS

11 STRUCTURE UPLOADED

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SAMPLE SEARCH INITIATED 09:22:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 43 TO ITERATE

100.04 PROCESSED 43 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 467 TO 1253
PROJECTED ANSWERS: 3 TO 163

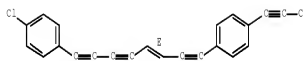
12 3 SEA SSS SAM L1

=> d scan

12 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-

dimethylethyl]dimethylsilyl]oxy)methyl]-6-(4-iodophenyl)-3-hexene-1,5-
 diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-
 [(trimethylsilyl)ethynyl]-, (6E)- (9CI)
 MF C55 H85 I O4 Si5

Double bond geometry as shown.



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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

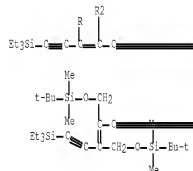
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
 IN Copper(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-
 dimethylethyl]dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-
 diynyl]disiprido[3,2-a:2',3'-c]phenazine-KM4,KM5]-, (T-4)-,
 bis[hexafluorophosphate(1-)] (9CI)
 MF C140 H212 Cu N8 O8 Si12 . 2 F6 P

CM 1

PAGE 1-A

PAGE 1-B



1

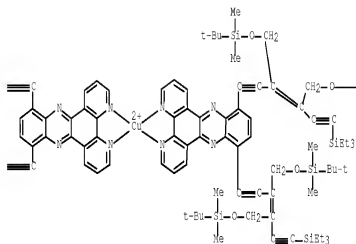
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN INDEX NAME NOT YET ASSIGNED
 MF C22 H10 Cl2

Double bond geometry as shown.

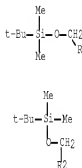
PAGE 1-B



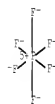
PAGE 1-C



PAGE 2-A



CM 2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l1 sss full
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FULL SCREEN SEARCH COMPLETED - 765 TO ITERATE

100.04 PROCESSED 765 ITERATIONS 49 ANSWERS
SEARCH TIME: 00.00.01

13 49 SEA SSS FUL L1

=> file caplus
C
=> s 13
14 15 L3

=> d itik abs hitetr 1-
YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/(N):y

14 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2009:1167697 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 151:470292
TITLE: Synthesis of hybrid masked triyne-phenylene axial rods containing (E)- β -chlorovinylsilanes in the π -conjugated framework
AUTHOR(S): Weller, Michael D.; Kariuki, Benson M.; Cox, Liam R.
CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK
SOURCE: Journal of Organic Chemistry (2009), 74(20), 7898-7907
CODEN: JOCEAH; ISSN: 0022-3243
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Silyl-masked hexayne Me3SiC.tpbond.CC(1:C(SiR3)C.tpbond.CC.tpbond.C(SiR3)C(1C.tpbond.CSiMe3 (7, SiR3 = tBuPh2Si) undergoes fluoride-induced β -elimination yielding, after terminal modifications, 1,12-diaryldodecahexaynes; compared to its positional isomer Me3SiC.tpbond.CC(SiR3)C(1C.tpbond.CC.tpbond.CC(1:C(SiR3)C.tpbond.CSiMe3 (2, same SiR3), prepared earlier, the compound 7 provides increased flexibility, allowing introduction of aromatic spacer groups, useful in production of carbyne-type mol. wires. A two-directional synthesis of a masked hexayne 7, in which two β -chlorovinylsilanes protect two of the internal alkynes, is reported. The key step involves the Pd-catalyzed oxidative dimerization of alkyne HC.tpbond.CC(SiR3)C(1C.tpbond.CC(20THP (10) to

provide diyne TPEOCH2C1:C(SiR3)C.tpbond.CC.tpbond.CC(SiR3):CC1CH2OTHP (12), which is elaborated into centrosym. masked hexayne 7 in four steps. Masked hexayne 7 is a constitutional isomer of masked hexayne 2, which has been used as a monomer unit for oligoyne assembly. Although masked hexayne 7 was not as convenient a building block as 2 for application in oligoyne assembly, one of its precursors, namely alkyne 10, could be used successfully in Sonogashira couplings, which allowed the incorporation of aromatic spacers and the formation of hybrid masked triyne-phenylenes

Me3SiC.tpbond.CC1:C(SiR3)C.tpbond.C-1,4-C6H4C.tpbond.CC(SiR3):CC1C.tpbond.CSiMe3 (20) and [Me3SiC.tpbond.CC1:C(SiR3)C.tpbond.C-1,4-C6H4C.tpbond.C]2 (28). Comps. 20 and 28 both contain removable end-groups, which will permit their application as building blocks for the assembly of classes of long-chain, π -conjugated rod-like mols. Rod-like mol.

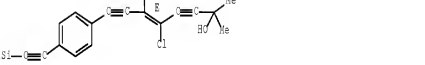
Me2C(OH)C.tpbond.CC1:C(SiR3)C.tpbond.CC6H4C.tpbond.C]2C(SiR3):CC1C.tpbond.CCMe2(OH) (34, C6H4 = 1,4-phenylene), which possesses a similar conjugated scaffold as 28, was also prepared by using a similar strategy. Treatment of 34 with TBAF effected a 2-fold dechlorosilylation to provide a rigid rod mol. Me2C(OH)C.tpbond.C]3C6H4(C.tpbond.C)2C6H4(C.tpbond.C)3CMe2(OH) (35) in which two 1,4-phenylene units interrupt an octayne scaffold.

IT 1131033-44-3P 1131033-45-4P 1131033-46-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of π -conjugated p-phenylene-bridged β -chloro silyl-substituted enynes as precursors for arylene-containing polyene mol. wires)

RN 1191093-44-3 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



Me3Si- (terminal group)

RN 1191093-45-4 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



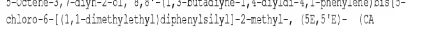
Me3Si- (terminal group)

RN 1191093-46-5 CAPLUS

CN 5-Octene-3,7-diyn-2-yl, 8,8'-[(1,3-butadiene-1,4-diyl)-4,1-phenylene]bis[5-chloro-6-[(1,1-dimethylethyl)diphenylsilyl]-2-methyl-, (5E,5'E)- (CA

INDEX NAME)

Double bond geometry as shown.



Me3Si- (terminal group)

RN 1191093-47-6 CAPLUS

CN 5-Octene-3,7-diyn-2-yl, 8,8'-[(1,3-butadiene-1,4-diyl)-4,1-phenylene]bis[5-chloro-6-[(1,1-dimethylethyl)diphenylsilyl]-2-methyl-, (5E,5'E)- (CA

INDEX NAME)

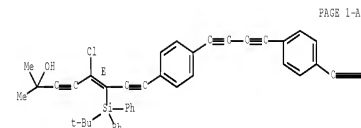
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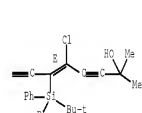
Me3Si- (terminal group)

INDEX NAME)

Double bond geometry as shown.



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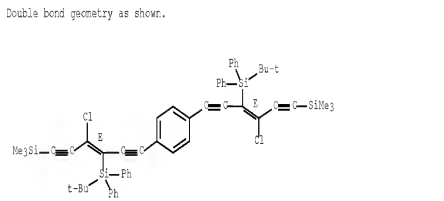
IT 1131093-33-7P 1131093-41-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of π -conjugated p-phenylene-bridged β -chloro silyl-substituted enynes as precursors for arylene-containing polyene mol. wires)

RN 1191093-33-0 CAPLUS
 CN Benzene, 1,4-bis[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



Me3Si- (terminal group)

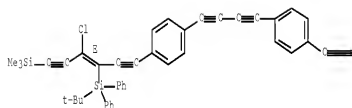
RN 1191093-41-0 CAPLUS

CN Benzene, 1,4-bis[(1,3-butadiene-1,4-diyl)bis[4-[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

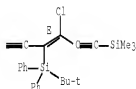
Double bond geometry as shown.



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PAGE 1-B



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 2005:1004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNED(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

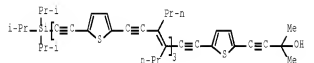
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, ST, TJ, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
FW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AG, AI, AU, BG, BR, CA, CH, CN, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, NG, TD, TG				
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPL. INFO.:			JP 2004-65446	A 20040309



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 864684-31-1P 864684-31-UP
 RL: IMP (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREF (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of π -conjugated aromatic ring-containing acetylene

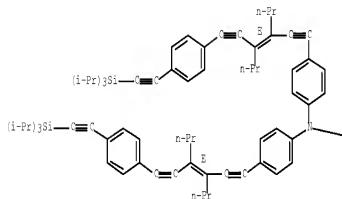
derivs. as organic electroluminescent devices)

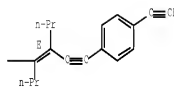
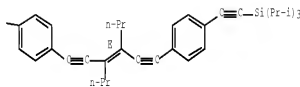
RN 864684-31-1 CAPLUS

CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-(4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A





RN 864684-32-2 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 864684-21-92 864684-22-06 864684-23-1P

864684-24-2P 864684-25-3E 864684-26-4P

864684-27-5P 864684-28-6P 864684-29-7P

864684-30-8P 864684-31-9P

RI: DEV (Device component use); IMF (Industrial manufacture); SEN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

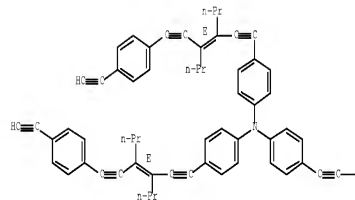
(preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 864684-21-9 CAPLUS

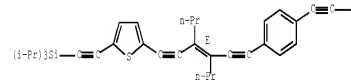
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diy-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

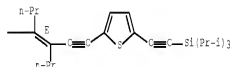
PAGE 1-A



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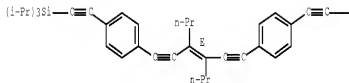
RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-

methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

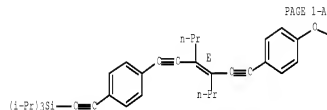
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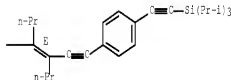
CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis(tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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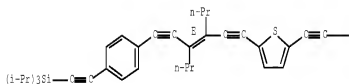


RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

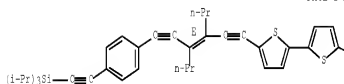


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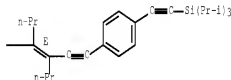
CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

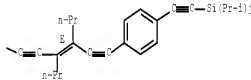
PAGE 1-A



PAGE 1-B



PAGE 1-B

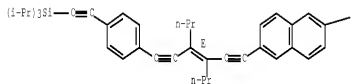


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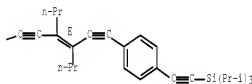
CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

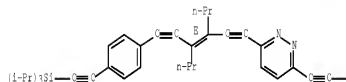


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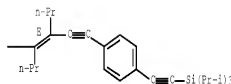
CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

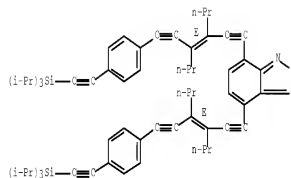


RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

1-yl]- (CA INDEX NAME)

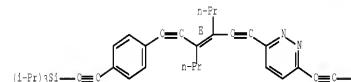
Double bond geometry as shown.



RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

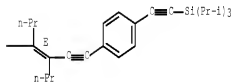
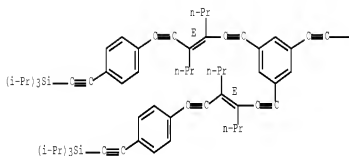
Double bond geometry as shown.



RN 864684-30-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

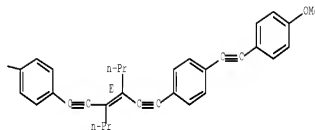
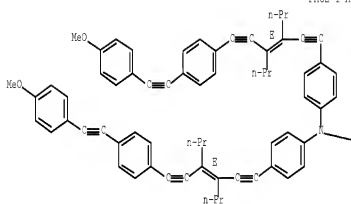
Double bond geometry as shown.



RN 864684-33-3 CAPLUS

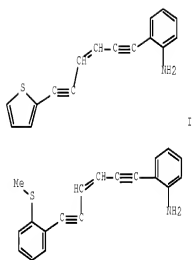
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-{4-[2-(4-methoxyphenyl)ethynyl]phenyl}ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-{4-[2-(4-methoxyphenyl)ethynyl]phenyl}ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-{4-[2-(4-methoxyphenyl)ethynyl]phenyl}ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2005:354187 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 143:333
 TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diynes, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivatives
 AUTHOR(S): Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575
 CODEN: BMCEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:333
 GI



AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from 0.01 to 96.6 μ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10⁻⁷M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(2)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 852619-13-7P

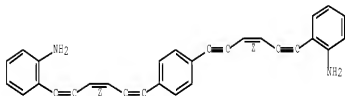
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(2)-hexen-1,5-diyne, 2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their derivs.)

RN 852619-13-7 CAPLUS

CN Benzenamine, 2,2'-(1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl)bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 200511022 CAPLUS Full-text
 DOCUMENT NUMBER: 142:113747
 TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents
 INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong
 PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan
 SOURCE: U.S. Pat. Appl. Publ., 41 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FILING ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050004212	A1	20050106	US 2004-847667	20040518
US 7332623	B2	20080219		
CA 2570366	A1	20050317	CA 2004-2570366	20040909
WO 2005023131	A2	20050317	WO 2004-US29334	20040909
WO 2005023131	A3	20050512		
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WO 2005023145 A2 20050317 WO 2004-US29337 20040909
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 RU 2336846 C2 20081027 RU 2006-106623 20040909
 RU 2341229 C2 20081220 RU 2006-106621 20040909
 CA 2540119 C 20090331 CA 2004-2540119 20040909
 RU 2352321 C2 20090420 RU 2006-106392 20040909
 RU 2368349 C1 20090927 RU 2008-106521 20040909
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 IN 20060071964 A 20070810 IN 2006-DN1964 20060410
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 US 2003-463870 P 20030630
 US 2003-501269 P 20030909
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 US 2004-847429 A 20040517
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 WO 2004-US29335 W 20040909
 WO 2004-US29336 W 20040909
 WO 2004-US29337 W 20040909
 WO 2004-US29338 W 20040909
 US 2006-488204 A1 20060718

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUI DISPLAY FORMAT

OTHER SOURCE(S): NARGENT 142:113747

GI



Q=



Q1=

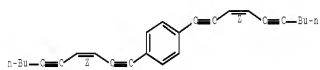


AB This invention provides aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts or solvates thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxyethyl, tetrahydropyranyloxypropyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). These compds. found to have inhibitory activities against topoisomerase I or act as a S phase or G2/M phase blocker and were also tested in vitro in anticancer assay. 4-((1Z)-3-Dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((1Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

IT 4579(1)-25-79
 RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BICI (Biological study); PRP (Preparation); USES (Uses)
 (preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)
 RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di(3(2)-3-decene-1,5-diyn-1-yl-) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS APPEAR IN THE RE FORMAT

L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2005:15944 CAPLUS Full-text

DOCUMENT NUMBER: 142:113746

TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents and pharmaceutical compositions comprising them

Wu, Ming-Jung; Lin, Chi-Fong

PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan

SOURCE: U.S. Pat. Appl. Publ., 41 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 20050004211	A1	20050106	US 2004-847659	20040518
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CA 2570366	A1	20050317	CA 2004-2570366	20040909
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WO 2005023131	A3	20050512		
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WO 2005023144	A2	20050317	WO 2004-US29335	20040909
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WO 2005023144	A2	20050317	WO 2004-US29336	20040909
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WO 2005023144 A3 20050512

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WO 2005023145	A2	20050317	WO 2004-US29337	20040909
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WO 2005023145 A3 20050512

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WO 2005023146	A2	20050317	WO 2004-US29338	20040909
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WO 2005023146 A3 20050512

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RW: BM, GE, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GW, GQ, GM, ML, MR, NE, NI, TD, TG

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RU 2322215	C2	20080420	RU 2006-106393	20040909
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RU 2329007	C2	20080720	RU 2006-106622	20040909
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RU 2336846	C2	20081027	RU 2006-106623	20040909
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 JP 2009183753 A 20090820 JP 2009-125481 20090525

PRIORITY APPLN. INFO.:

US 2003-483887P P 20030630
 US 2003-501266P P 20030909
 US 2004-832168 A 20040426
 US 2004-842302 A 20040510
 US 2004-847429 A 20040517
 US 2004-887644 A 20040709
 US 2004-887667 A 20040709
 US 2004-888206 A 20040709
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 WO 2004-US29334 W 20040909
 WO 2004-US29335 W 20040909
 WO 2004-US29336 W 20040909
 WO 2004-US29337 W 20040909
 WO 2004-US29338 W 20040909
 US 2006-488204 A1 20060718

OTHER SOURCE(S): MARPAT 142:113746
 GI



Q=



Q1=



AB A pharmaceutical compns. comprises aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxyethyl, tetrahydropyranyloxypropyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). The pharmaceutical composition is used to treat a subject afflicted with a tumor/cancer by inhibiting topoisomerase I activities or blocking the S phase or G2/M phase of the tumor/cancer cells. The tumor/cancer cell is selected from leukemia cancer cells, non-small-cell lung cancer cells, col on cancer

cells, CNS cancer cells, melanoma cancer cells, ovarian cancer cells, renal cancer cells, prostate cancer cells and breast cancer cells. These compds. were tested in vitro for inhibitory activities against topoisomerase I, cell cycle at a S phase or G2/M phase blocker, and anticancer growth. For example, 4-((Z)-3-Dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

II

RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BICL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)

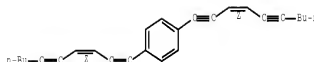
RN

457914-65-7 CAPLUS

CN

Benzene, 1,4-di(3Z)-3-decane-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



CS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

14 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2004:480115 CAPLUS Full-text
 DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

AUTHOR(S): Nakano, Yuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuki; Sato, Fumie
 DEPARTMENT OF BIOMOLECULAR ENGINEERING, TOKYO INSTITUTE OF TECHNOLOGY, MIDORI, YOKOHAMA, KANAGAWA, 226-8501, JAPAN

SOURCE: Organic Letters (2004), 6(14), 2373-2376
 CODEN: ORLEF7; ISSN: 1523-7060

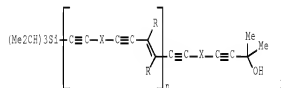
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

GI



AB Synthesis and fluorescence properties of π -conjugated compds. I ($n = 1 - 3$; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

PAGE 1-B

II 740810-61-14 740810-62-2P

RI: PRE (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and absorption and fluorescence spectra of conjugated

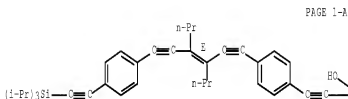
oligomers

having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-61-1 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-(2-[4-(2-[tris(1-methylethyl)silyl]ethynyl)phenyl]ethynyl)-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



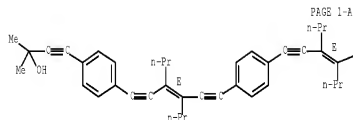
PAGE 1-B



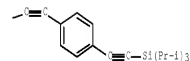
RN 740810-62-2 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[(4-[(3E)-3-propyl-4-[(4-[(tris(1-methylethyl)silyl]ethynyl)phenyl]ethynyl)-3-hepten-1-yn-1-yl]phenyl]ethynyl)-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-C



II 740810-63-3P

RI: PRE (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and absorption and fluorescence spectra of conjugated

oligomers

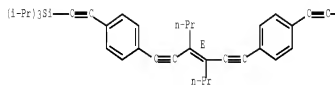
having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-63-3 CAPLUS

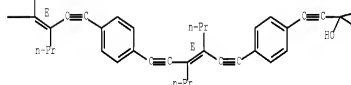
CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[(4-[(3E)-3-propyl-4-[(4-[(3E)-3-propyl-4-[(4-[(tris(1-methylethyl)silyl]ethynyl)phenyl]ethynyl)-3-hepten-1-yn-1-yl]phenyl]ethynyl)-3-hepten-1-yn-1-yl]phenyl]ethynyl)-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

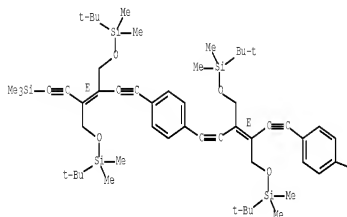


OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS
RECORD (20 CITINGS)
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Double bond geometry as shown.

PAGE 1-A

14 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2004:320526 CAPLUS Full-text
DOCUMENT NUMBER: 141:54000
TITLE: Solid-phase synthesis of oligo(triacetylene)s and
oligo(phenylenetriacetylene)s employing Sonogashira
and Cadiot-Chodkiewicz-type cross-coupling reactions
AUTHOR(S): Utesch, Nils F.; Diederich, Francois; Boudon, Corinne;
Gisselbrecht, Jean-Paul; Gross, Maurice
CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg,
HCI, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718
CODEN: HCACNV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:54000



AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse
oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-
Chodkiewicz-type cross-couplings as the key steps in the construction of the
acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-
iodophenyl)triazene linker was chosen as the polymeric support. The linker
selection was made based on the results of several model studies in the liquid
phase. For the solid-support synthesis of p-
1[CH4C.tpbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tpbond.C]nSiMe3 [I, n =
2-4] a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira
cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii)
cleavage of the linker with liberation of I. The longest-wavelength absorption
maxima of I [n = 1-4] shift bathochromically with increasing oligomeric
length, from λmax 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the
electronic absorption data, the effective conjugation length (ECL) of the
oligo(phenylene triacetylene)s is estimated to involve at least four monomer
units and 40 C-atoms. π-Electron conjugation in these oligomers is less
efficient than in
Me3Si[CH4C.tpbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tpbond.C] nSiMe3 (II)
due to poor transmittance of π-electron delocalization by the Ph rings
inserted into the oligomeric backbone. Similar conclusions were drawn from
the electrochem. properties of the two oligomeric series as determined by
cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are
strongly fluorescent, with the highest quantum yield ΦF = 0.69 measured for I
[n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded
smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions
employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be
developed.

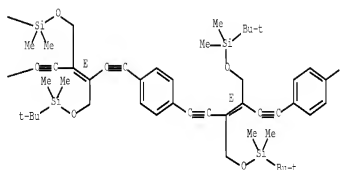
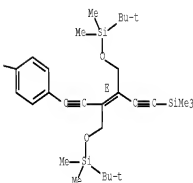
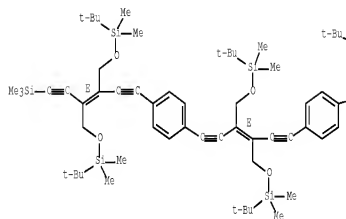
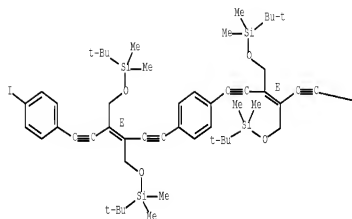
PAGE 1-B

II 554459-62-0P 554459-63-1P 114416-64-2W
RL: PRP (Properties); SW: Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of oligo(triacetylene)s and
oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz
cross-coupling reactions)

RN 554459-62-0 CAPLUS
CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-
dimethylethyl]dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-
diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-

RN 554459-63-1 CAPLUS
CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-(4-[(3E)-3,4-bis[[[(1,1-
dimethylethyl]dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-
diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-
[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

II 704916-29-0P

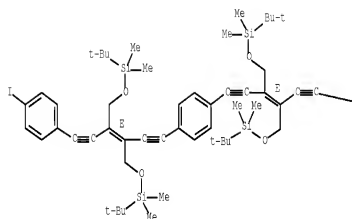
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadot-Chodkiewicz cross-coupling reactions)

RN 704916-29-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[[4-(iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.



of a central heterospacer group between two (E)-hex-3-ene-1,5-diyne moieties. A significant increase in the 2nd hyperpolarizability χ is expected if the central spacer fragment is an extended conjugated chromophore. The authors present mol.s. with enhanced 2nd hyperpolarizability caused by the presence of highly conjugated spacer groups, which increase the overall π -electron delocalization. Some metal complexes obtained from the coordination of these hybrid oligomers to transition-metal centers also were studied and revealed substantial differences in the capacities of the metal centers to act as electronic bridges. Finally, theor. predictions of the relative differences in the 2nd hyperpolarizabilities of the new spacer compds. are in good agreement with the exptl. results.

IT 628738-17-0 628738-19-2 628738-25-5

RI: PRP (Properties)

(third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores)

RN 628738-17-0 CAPLUS

CN Quinoxaline, 5,8-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyne]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2003:592887 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:20929

TITLE: Third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores

AUTHOR(S): Conclio, S.; Biaggio, I.; Gunter, P.; Piatto, S. P.; Edelman, M. J.; Raimundo, J.-M.; Diederich, F.

CORPORATE SOURCE: Swiss Federal Institute of Technology, Institute of Quantum Electronics, Nonlinear Optics Laboratory, ETH-Honggerberg, Zurich, CH-8093, Switz.

SOURCE: Journal of the Optical Society of America B: Optical Physics (2003), 20(8), 1656-1660

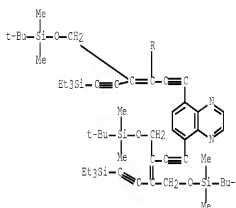
CODEN: JOBPDE; ISSN: 0740-3224

PUBLISHER: Optical Society of America

DOCUMENT TYPE: Journal

LANGUAGE: English

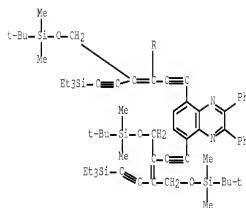
AB A new approach to tuning the nonlinear optical properties of hybrid oligo(triacetylene) compds. was studied. The method is based on the insertion



RN 628738-19-2 CAPLUS

CN Quinoxaline, 5,8-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyne]-1-yl]-2,3-diphenyl- (CA INDEX NAME)

PAGE 1-A

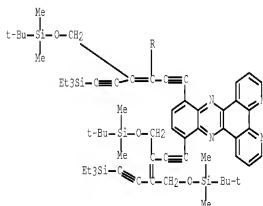


PAGE 2-A



RN 628738-20-5 CAPLUS

CN Dipyrido[3,2-a:2',3'-c]phenazine, 10,13-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (SCI) (CA INDEX NAME)



PAGE 1-A

PAGE 2-A



CS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2003:23491 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 139:85055
TITLE: Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadot-Chodkiewicz-type cross-coupling reactions
AUTHOR(S): Utesch, Wils F.; Diederich, Francois
CORPORATE SOURCE: Laboratorium für Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.
SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239
CODEN: OBCHAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:85055

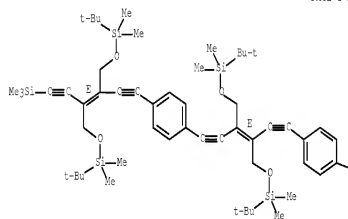
AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., 1[4-C6H4C.tplbond.CCR:CCR.tplbond.C]nSiMe3 (R = CH2CSiBuMe2, n = 1, 2, 3, 4) members of a new class of linearly π -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

IT 554459-62-PP 554459-63-PP 554459-64-ZF
RL: PRP (Properties); SPW (Synthetic preparation); PREP (Preparation) (electronic absorption and emission, UV/VIS spectra);
poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)
RN 554459-62-0 CAPLUS

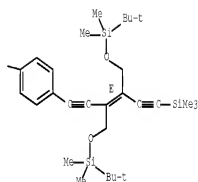
CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E)- (SCI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

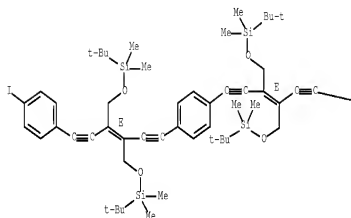


RN 554459-63-1 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-([4-((3E)-6-(4-((3E)-3,4-bis(((1,1-dimethylethyl)dimethylsilyl)oxy)methyl)-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl)-3,4-bis(((1,1-dimethylethyl)dimethylsilyl)oxy)methyl)-3-hexene-1,5-diynyl]phenyl)ethynyl)-2,2,3,3,10,10,11,11-octamethyl-7-((trimethylsilyl)ethynyl)-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

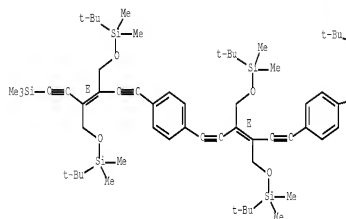


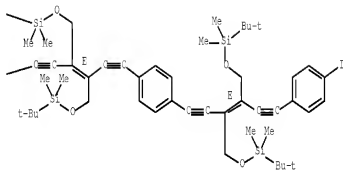
RN 554459-64-2 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-([4-((3E)-6-(4-((3E)-3,4-bis(((1,1-dimethylethyl)dimethylsilyl)oxy)methyl)-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl)-3,4-bis(((1,1-dimethylethyl)dimethylsilyl)oxy)methyl)-3-hexene-1,5-diynyl]phenyl)ethynyl)-7-([4-((3E)-3,4-bis(((1,1-dimethylethyl)dimethylsilyl)oxy)methyl)-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl)ethynyl)-2,2,3,3,10,10,11,11-octamethyl-1-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



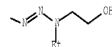
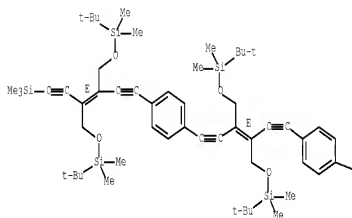


IT 554459-71-109, Merrifield resin-supported
 554459-72-109, Merrifield resin-supported 554459-73-109
 , Merrifield resin-supported
 RI: RCT (Reactant); SPN (Synthetic preparation); PRPZ (Preparation); RACT
 (Reactant or reagent)
 (preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed
 cross-coupling reactions of supported poly(triacetylene)-derived
 oligomers)

RN 554459-71-1 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

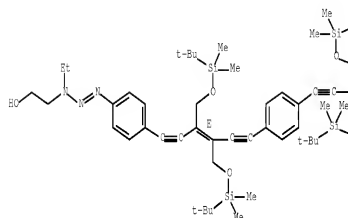
Double bond geometry as described by E or Z.

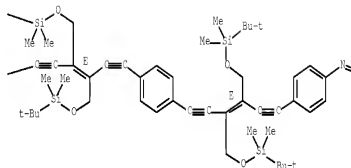
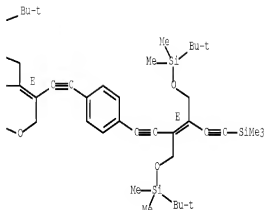


RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.





RN 554459-73-3 CAPLUS

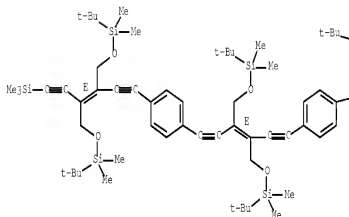
CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

PAGE 1-C

Double bond geometry as described by E or Z.



PAGE 1-A



CS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)
 REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2002:719354 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 138:25161
 TITLE: Third-order nonlinear optical properties of in-backbone substituted conjugated polymers
 AUTHOR(S): Gubler, U.; Concilio, S.; Bosshard, Ch.; Biaggio, I.; Gunter, P.; Martin, R. E.; Edelmann, M. J.; Wytke, J. A.; Diederich, F.
 CORPORATE SOURCE: Institute of Quantum Electronics, ETH-Honggerberg, Zurich, CH-8033, Switz.
 SOURCE: Applied Physics Letters (2002), 81(13), 2322-2324
 CODEN: APPLAB; ISSN: 0003-6951
 PUBLISHER: American Institute of Physics
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB An alternative approach for tuning of the third-order nonlinear optical properties of organic mols. is based on insertion a functional group into the path of the π -electron conjugation instead of at chain ends. This scheme enhances the second-order hyperpolarizability for short mols., but in two instances where such mols. were polymerized into longer mols. the overall hyperpolarizability was lower. The study is based on tert-butyl(dimethylsiloxy)-vinyl-poly(triacetylene) as the basic linear conjugated polymer, with spacer of anthracene, benzene, naphthalene, thiophene,

tetramethylbenzene, furan tetrafluorobenzene, pyridine, biphenyl, pyrazine, and bis(triethylphosphine-Pt).

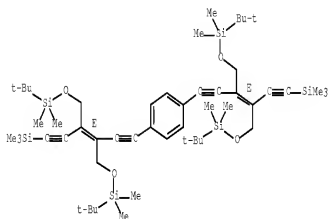
IT 249616-79-3 CAPLUS
 9,10-Bis[(E)-3,4-bis[(tert-butyl)dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]anthracene 249616-84-0
 249616-81-1, 1,4-Bis[(E)-3,4-bis[(tert-butyl)dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene

RU: FRP (Properties)

(role of in-backbone spacer on third-order nonlinear optical properties of polyacetylene conjugated polymers)

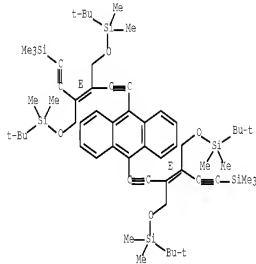
RN 249616-79-3 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylene)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



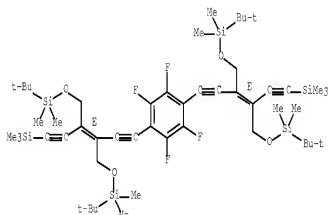
RN 249616-83-9 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(9,10-anthracenediyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



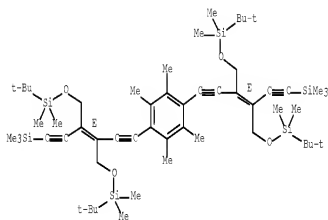
RN 249616-84-0 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,3,5,6-tetrafluoro-1,4-phenylene)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 249616-87-3 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,3,5,6-tetramethyl-1,4-phenylene)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
 REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

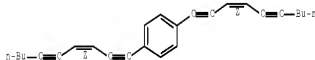
L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 ACS ON SIN
 ACCESSION NUMBER: 2002:700980 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:247934
 TITLE: Cytotoxicities and topoisomerase I inhibitory activities of 2-[2-(2-alkyrylphenyl)ethynyl]benzonitriles, 1-aryldec-3-ene-1,5-diyne, and related bis(enediynyl)arene compounds
 AUTHOR(S): Lin, Chi-Fong; Lu, Wen-Der; Hsieh, Pei-Chen; Kuo, Yao-Baur; Chiu, Huey-Fen; Wang, Chyi-Jia; Wu, Ming-Jung
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan
 SOURCE: Helvetica Chimica Acta (2002), 85(8), 2564-2575
 CODEN: HCACAV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:247934

AB The activities of a series of acyclic enediynes, 2-(6-substituted hex-3-ene-1,5-diynyl)benzonitriles (1-5) and their derivs. 7-23 were evaluated against several solid tumor cell lines and topoisomerase I. Comps. 1-5 show selective cytotoxicity with Hepa cells, and 2-(6-phenylhex-3-ene-1,5-diynyl)benzonitrile (5) reveals the most-potent activity. Analogs 8-10 and 13-22 also have the same effect with DLD cells; 1-[(1Z)-dec-3-ene-1,5-diynyl]-4-nitrobenzene (21) shows the highest activity among them. Moreover, 1-[(1Z)-dec-3-ene-1,5-diynyl]-2-(trifluoromethyl)benzene (20) exhibits the strongest inhibitory activity with the HeLa cell line. Derivs. 9, 10, 18, and 23 display inhibitory activities with topoisomerase I at 67 μM. The cell-cycle anal. of compound 5, which induces a significant blockage in S phase, indicates that these novel enediynes probably undergo other biol. pathways leading to the cytotoxicity, except the inhibitory activity toward topoisomerase I.

IT 457314-65-7P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOU (Biological study); PREP (Preparation); USES (Uses)
 (cytotoxicity and topoisomerase I inhibitory activity of 2-[2-(2-alkyrylphenyl)ethynyl]benzonitriles, 1-aryldec-3-ene-1,5-diyne, and related bis(enediynyl)arene compds.)
 RN 457914-65-7 CAPLUS
 CN Benzene, 1,4-di[(3Z)-3-dec-ene-1,5-diyn-1-yl]- (CA INDEX NAME)

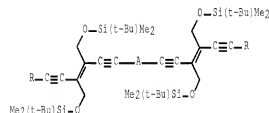
Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
 REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2002:628032 CAPLUS Full-text
 DOCUMENT NUMBER: 138:4578
 TITLE: Dramatically enhanced fluorescence of heteroaromatic

chromophores upon insertion as spacers into oligo(triacetylene)s
 Edelman, Michael J.; Raimundo, Jean-Manuel; Utesch, Nils F.; Diederich, Francois
 CORPORATE SOURCE: Lab. Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.
 SOURCE: Helvetica Chimica Acta (2002), 85(7), 2195-2213
 CODEN: HCACAV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:4578
 GI



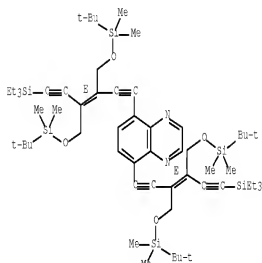
AB In continuation of a previous study on the modulation of π-electron conjugation of oligo(triacetylene)s by insertion of central hetero-spacer fragments between two (E)-hex-3-ene-1,5-diyne ((E)-1,2-diethynyl)ethane, DEE) moieties, trimeric hybrid oligomers (1; A = spacer, R = SiEt3, SiMe3) were prepared. Spacers used were both electron-deficient (quinoxaline-based heterocycles, pyridazine) and electron-rich (2,2'-bithiophene, 9,9'-diethyl-9H-fluorene)chromophores. With a dipyrrophenazine spacer, transition metal complexes were synthesized as potential precursors for nanoscale scaffolding based on both covalent acetylenic coupling and supramol. assembly. The UV/visible spectra revealed that the majority of spacers provided heterotrimers featuring extended π-electron delocalization. The new hybrid chromophores show a dramatically enhanced fluorescence compared with the DEE dimer and homo-trimer. This increase in emission intensity appears as a general feature of these systems: even if the spacer mol. is nonfluorescent, the corresponding hetero-trimer may show a strong emission. The redox properties of the new hybrid chromophores were determined by cyclic voltammetry (CV) and rotating disk voltammetry (RDV). In each case, the first 1-electron reduction step in the hetero-trimers appeared anodically shifted compared with DEE dimer and homo-trimer. With larger spacer chromophore extending into two dimensions, the anodic shift (by 240-490 mV) seems to originate from inductive effects of the two strongly electron-accepting DEE substituents rather than from extended π-electron conjugation along the oligomeric backbone, as had previously been observed for DEE substituted porphyrins.
 IT 477233-33-5P 477234-02-3P 477294-41-2P
 477294-02-3P 477294-46-5P 477234-06-7P
 477284-08-9P
 RL: CFS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROOC (Process)
 (preparation, electrochem. properties and dramatically enhanced fluorescence

of compds. consisting of heteroarom. chromophores inserted as spacers
into oligo(triacetylene)s)

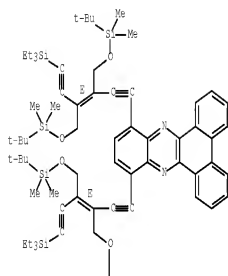
RN 477293-99-5 CAPLUS

CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



Double bond geometry as shown.

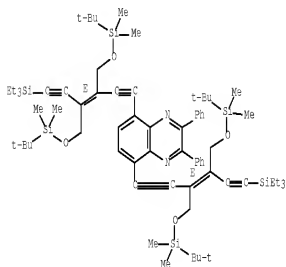


PAGE 1-A

RN 477294-00-1 CAPLUS

CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]-2,3-diphenyl- (CA INDEX NAME)

Double bond geometry as shown.



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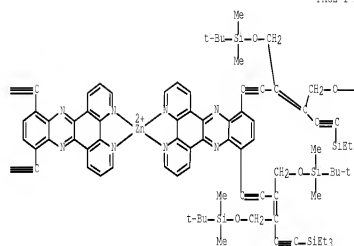
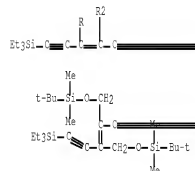
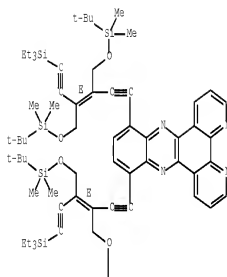
RN 477294-02-3 CAPLUS

CN Dipyrrodo[3,2-a:2',3'-c]phenazine, 10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 477294-01-2 CAPLUS

CN Dibenzo[a,c]phenazine, 10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (CA INDEX NAME)



RN 477294-04-5 CAPLUS
 CN Zinc(2+), bis[[10,13-bis-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-dienyl]dipyrido[3,2-a:2',3'-c]phenazine-4,8,15,20-tetrone], (T-4)], salt with trifluoromethanesulfonic acid (1:2) (PCI) (CA INDEX NAME)

CM 1

CRN 477294-03-4
 CMF C140 R212 W8 O8 S112 Zn
 CCI CCS



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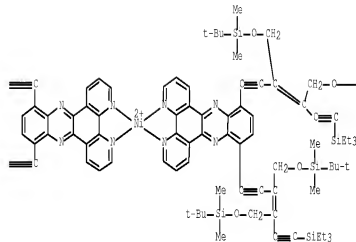
CM 2

CRN 37181-39-8

CME C F3 O3 S



PAGE 1-B



PAGE 1-C

RN 477294-06-7 CAPLUS

CN Nickel (2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexeno-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-K(4,K(5)-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 477294-05-6

CME C140 H212 N8 Ni O8 Si12

CCI CCS

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PAGE 2-A



CM 2

CRN 14797-73-0

CMF C1 04

PAGE 1-B



RN 477294-08-9 CAPLUS

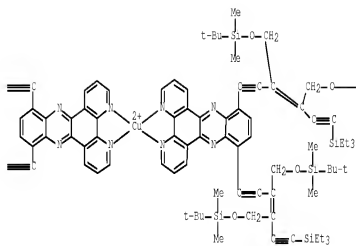
CN Copper (2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-κN4,κN5]-, (T-4)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 477294-07-8

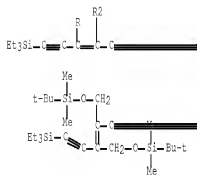
CMF C140 R212 Cu N8 O8 Si12

CCI CCS



PAGE 1-C

PAGE 1-A



PAGE 2-A



CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



OS.CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

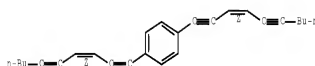
L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2009 ACS ON STN
 ACCESSION NUMBER: 2002:539072 CAPLUS Full-text
 DOCUMENT NUMBER: 137:232177
 TITLE: Anionic Cycloaromatization of 1-aryl-3-hexen-1,5-dienes Initiated by Methoxide Addition: Synthesis of Phenanthridinones, Benzo[c]phenanthridinones, and Biaryls
 AUTHOR(S): Wu, Ming-Jung; Lin, Chi-Fong; Lu, Wen-Der
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan
 SOURCE: Journal of Organic Chemistry (2002), 67(17), 5907-5912
 CCOCN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:232177

AB Treatment of 2-((Z)-6-substituted-3-hexene-1,5-diynyl)benzonitriles with sodium methoxide in refluxing methanol in the presence of a polar aprotic solvent, such as DMSO, HMPA, THF, or 18-crown-6, gave phenanthridinones in 21-77% yields. In these cases, addition of 10% DMSO into the reaction mixture gave the highest yield. On the other hand, methanolysis of 2-((Z)-6-alkynylphenyl)ethynyl)benzonitriles under the same reaction conditions gave benzo[c]phenanthridinones in 31-57% yields. Methanolysis of (Z)-1-aryl-3-hexen-1,5-dienes in the presence of 2 equiv of tetrabutylammonium iodide gave biaryls in 14-64% yields. It is found that the reactions with aryl groups bearing electron-withdrawing groups proceeded at greater rates and gave better yields.

IT 457914-65-7P
 RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (anionic cycloaromatization of 1-aryl-3-hexen-1,5-dienes initiated by addition of methanol)

RN 457914-65-7 CAPLUS
 CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

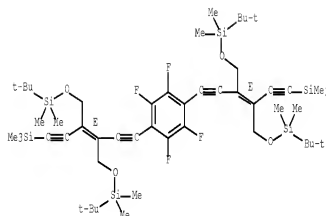
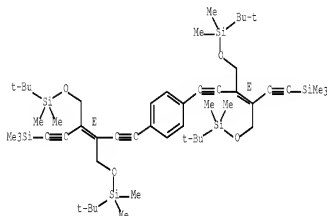
L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2009 ACS ON STN
 ACCESSION NUMBER: 1999:625317 CAPLUS Full-text
 DOCUMENT NUMBER: 131:337377
 TITLE: Modulation of π -electron conjugation in oligo(triacylene) chromophores by incorporation of a central spacer
 AUTHOR(S): Martin, Rainer E.; Wytko, Jennifer A.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice
 CORPORATE SOURCE: Laboratorium für Organische Chemie, ETH-Zentrum, Zurich, CH-8032, Germany
 SOURCE: Helvetica Chimica Acta (1999), 82(9), 1470-1485
 CCOCN: HCACAN; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of trimeric hybrid oligomers was prepared by insertion of different hetero-spacers between two (E)-hex-3-ene-1,5-diyne (E = 1,2-diethynylhexane, DEE) moieties, and the optical and electrochem. properties of the resulting π -conjugated materials were compared to those of the DEE dimer and trimer, which formally contain a DEE moiety as homo-spacer. The hetero-spacers were: benzenoid (phenylene, naphthalene, biphenylene, anthracene), π -electron-deficient (pyrazine, pyridine) and π -electron-rich (thiophene, furan) aromatic rings, and trans-Pt(PPh₃)₂. The hybrid oligomers were synthesized using the method of K. Sonogashira et al. (1978), i.e., cross-coupling between mono-protected DEE and the appropriately bis-functionalized spacer. UV/VIS data revealed that the majority of the hetero-spacers were less effective than the homo-spacer DEE in facilitating π -electron delocalization along the linearly conjugated oligomeric backbone. With increasing degree of benzenoid aromaticity in the hetero-spacer, the electronic communication between the terminal DEE moieties in the hybrid oligomers was reduced. As a remarkable exception, a large bathochromic shift of the longest-wavelength absorption maximum, which is indicative of enhanced π -electron delocalization, was obtained upon introducing an anthracene-9,10-diyl moiety as hetero-spacer. Electrochem. studies by cyclic and steady-state voltammetry confirmed the limited extent of π -electron delocalization in the majority of the hybrid oligomers. The fluorescence properties of many of the DEE hybrid materials were dramatically enhanced upon incorporation of the heterospacers. The heterocyclic derivs. containing pyridine, pyrazine, or thiophene spacers, resp., displayed a strong fluorescence emission, demonstrating the value of combining repeat units to modulate oligomeric and polymeric properties. The pyridine derivative provided an interesting example of a mol. system, in which both the electronic absorption and emission characteristics can be reversibly switched as a function of pH.
 IT 24916:18-38, 4-Bis[(E)-3,4-bis(((tert-butyl)dimethylsilyloxy)methyl)-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]benzene 24:16:18-38-38, 9,10-Bis[(E)-3,4-bis(((tert-butyl)dimethylsilyloxy)methyl)-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]anthracene 24:16:18-38-38, 24:16:18-38-38, 1,4-Bis[(E)-3,4-bis(((tert-butyl)dimethylsilyloxy)methyl)-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene
 RI: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and modulation of π -electron conjugation in oligoacetylene chromophores by central spacer with variable electron d.)

RN 249616-79-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

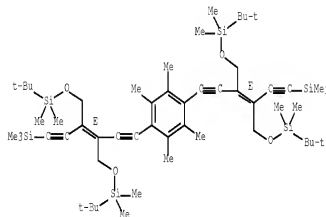
Double bond geometry as shown.



RN 249616-87-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

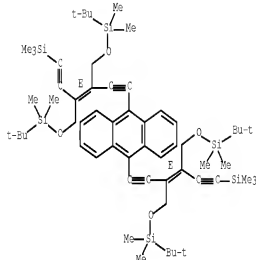
Double bond geometry as shown.



RN 249616-83-9 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(9,10-anthracenediyl)di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS RECORD (29 CITINGS)
REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:73330 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 68:78330

ORIGINAL REFERENCE NO.: 68:15123a,15126a

TITLE: Interaction of diiodoethylene with copper acetylides

AUTHOR(S): Ukhin, L. Yu.; Sladkov, A. M.; Gorskikh, V. I.

CORPORATE SOURCE: Inst. Elementorg. Soedin, Moscow, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1968), 4(1), 25-7

CODEN: ZORRAB; ISSN: 0514-7432

DOCUMENT TYPE: Journal

LANGUAGE: Russian

RN 249616-84-0 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

AB Reaction of trans-diiodoethylene (I) with Cu acetylides gave the condensation products of general formula RC.tpbond.CCH:CHI (IIa) or RC.tpbond.CCH:CHC.tpbond.CR (IIb). The structure of products was confirmed by ir and mass spectroscopy; trans configuration of the double bond was preserved. For example, a mixture of 3.23 g. (PhC.tpbond.C)2Cu, 2.78 g. I, and 100 ml. EtOMe2 was stirred 4 hrs. at 90° and then refluxed 2 hrs. Cooling, filtration, and addition of H2O to the filtrate precipitated 56% IIb (R = Ph) m. 111-12° (heptane). Similarly, IIb (R = Bu) b4 117°, nD20 1.5173 was prepared. Boiling 23.4 g. (BuC.tpbond.C)2Cu with 44.8 g. I in 125 ml. pyridine for 10 min. gave 40% IIa (R = Bu) b5 94-5°, nD20 1.5519. Similarly IIa (R = Ph) b2.5 112-14°, nD20 1.6080 was prepared. However boiling (p-ClC6H4C.tpbond.C)2Cu, with I in pyridine gave IIa (R = p-ClC6H4) m. 125-30° and IIb (R = p-IC6H4) m. 245-7° (C6H6-heptane), separated by crystallization. Also (p-ClC6H4C.tpbond.C)2Cu and I gave IIa (R = p-ClC6H4C.tpbond.C) m. 80-5° and IIb (R = p-ClC6H4C.tpbond.C) m. 179-85° (heptane). To further confirm the structures of IIa and IIb they were converted to boranes by refluxing with an excess of decaborane in PhMe solution. The following were characterized (compound, % yield, and m.p. given): 1,2-bis(1-butylbarany)ethylerane, 62, 153-5° (PhMe); 1-(β-iodovinyl)-2-phenylbarane, -, 227-35° (hexane); 1-(β-iodovinyl)-2-butylbarane, -, 72-4°.

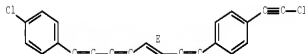
IT 1082663-34-02

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Interaction of diiodoethylene with copper acetylides)

RN 1082663-94-0 CAPLUS

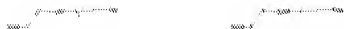
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



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chain nodes :
1 2 3 4 5 6 7 8 9

chain bonds :
1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9
exact/norm bonds :
6-7 7-8
exact bonds :
1-2 2-3 3-4 4-5 5-6 8-9

Cl:Cb,Cy,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS

15 STRUCTURE UPLOADED

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SAMPLE SEARCH INITIATED 09:41:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 408 TO ITERATE

100.04 PROCESSED 408 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

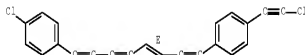
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROTECTED ITERATIONS: 6949 TO 9371
PROTECTED ANSWERS: 4 TO 200

16 4 SEA SSS SAM 15

=> d scan

16 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C22 H10 Cl2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

16 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Zinc(2+), [[diethyl 4,4'-[[10,20-bis((3E)-3,4-bis[[[1,1-dimethyl[ethyl]dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl-κN21,κN22,κN23,κN24]]bis(4,1-

MF C90 H124 N4 O10 Si6 Zn

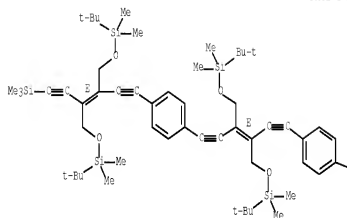
—08t

$$\begin{array}{c} \text{Me}_3\text{Si}-\text{C}\equiv\text{C}-\text{C}(\text{Me})_2-\text{CH}_2-\text{O}-\text{Si}(\text{Me})_2-\text{Bu-t} \\ \text{R} \\ \text{CH}_2-\text{O}-\text{Si}(\text{Me})_2-\text{Bu-t} \end{array}$$

CM 1

[illegible]

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1



CM 2



-I

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 15 sss full
 FULL SEARCH INITIATED 09:41:46 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 7813 TO ITERATE

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on SIN
 IN 4,9-Dicxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diylnyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI)
 MF C55 H85 I O4 Si5

Double bond geometry as shown.

100.04 PROCESSED 7813 ITERATIONS 123 ANSWERS
 SEARCH TIME: 00.00.01

17 123 SEA SSS FUL 15

=> file caplus

=> s 17
 18 39 L7

=> d ibib abs hitetr 1-
YOU HAVE REQUESTED DATA FROM 39 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 20091167687 CAPLUS Full-text

DOCUMENT NUMBER: 151:470282

TITLE: Synthesis of hybrid masked triyne-phenylene axial rods containing (E)- β -chlorovinylsilanes in the π -conjugated framework

AUTHOR(S): Weller, Michael D.; Kariuki, Benson M.; Cox, Liam R.

CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK

SOURCE: Journal of Organic Chemistry (2009), 74(20), 7898-7907

COCODE: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Silyl-masked hexayne Me3SiC.tpbond.CC(Cl)(SiR3)C.tpbond.CC.tpbond.C(SiR3)C.tpbond.CSiMe3 (7, SiR3 = t-BuPh2Si) undergoes fluoride-induced β -elimination yielding, after terminal modifications, 1,12-diaryldodecahexaynes; compared to its positional isomer

Me3SiC.tpbond.CC(SiR3)C(Cl)C.tpbond.CC.tpbond.C(Cl)(SiR3)C.tpbond.CSiMe 3 (2, same SiR3), prepared earlier, the compound 7 provides increased flexibility, allowing introduction of aromatic spacer groups, useful in production of carbyne-type mol. wires. A two-directional synthesis of a masked hexayne 7, in which two β -chlorovinylsilanes protect two of the internal alkynes, is reported. The key step involves the Pd-catalyzed oxidative dimerization of alkyne HC.tpbond.CC(SiR3)C(Cl)C2OTHP (10) to provide diyne THOCH2C(Cl)(SiR3)C.tpbond.CC.tpbond.CC(SiR3)C(Cl)C2OTHP (12), which is elaborated into centrosym. masked hexayne 7 in four steps. Masked hexayne 7 is a constitutional isomer of masked hexayne 2, which has been used as a monomer unit for oligoene assembly. Although masked hexayne 7 was not as convenient a building block as 2 for application in oligoene assembly, one of its precursors, namely alkyne 10, could be used successfully in Sonogashira couplings, which allowed the incorporation of aromatic spacers and the formation of hybrid masked triyne-phenylenes

Me3SiC.tpbond.CC(Cl)(SiR3)C.tpbond.C-1,4-C6H4C.tpbond.CC(SiR3)C(Cl)C.tpbond.CSiMe3 (20) and [Me3SiC.tpbond.CC(Cl)(SiR3)C.tpbond.C-1,4-C6H4C.tpbond.C]2 (28). Comps. 20 and 28 both contain removable end-groups, which will permit their application as building blocks for the assembly of classes of long-chain, π -conjugated rod-like mols. Rod-like mol.

Me2C(OH)C.tpbond.CC(Cl)(SiR3)C.tpbond.CC6H4C.tpbond.C]2C(SiR3)C(Cl)C.tpbond.CCMe2(OH) (34, C6H4 = 1,4-phenylene), which possesses a similar conjugated scaffold as 28, was also prepared by using a similar strategy. Treatment of 34 with TBAF effected a 2-fold dechlorosilylation to provide a rigid rod mol. Me2C(OH)C.tpbond.C]3C6H4(C.tpbond.C]2C6H4(C.tpbond.C]3CMe2(OH) (35) in which two 1,4-phenylene units interrupt an octayne scaffold.

IT 1191093-44-3P 1191093-45-4P 1191093-46-5P

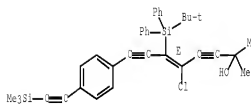
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of π -conjugated p-phenylene-bridged β -chloro silyl-substituted enynes as precursors for arylene-containing polyyne mol. wires)

RN 1191093-44-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

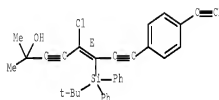
Double bond geometry as shown.



RN 1191093-45-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.

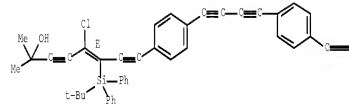


RN 1191093-46-5 CAPLUS

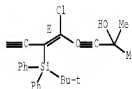
CN 5-Octene-3,7-diyne-2-ol, 8,8'-(1,3-butadiene-1,4-diyl)-4,1-phenylenebis[5-chloro-6-((1,1-dimethylethyl)diphenylsilyl)-2-methyl-, (5E,5'E)] - (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



IT 1191093-43-4P 1191093-41-4P

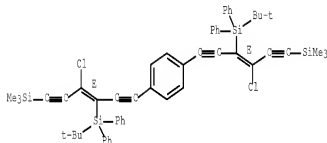
RE: SPN (Synthetic preparation); PREP (Preparation)

(preparation of π -conjugated p-phenylene-bridged θ -chloro silyl-substituted enynes as precursors for arylene-containing polyene mol. wires)

RN 1191093-33-0 CAPLUS

CN Benzene, 1,4-bis[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

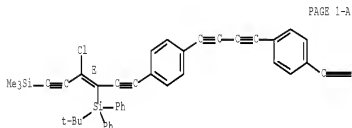
Double bond geometry as shown.



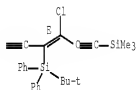
RN 1191093-41-0 CAPLUS

CN Benzene, 1,1'-[1,3-butadiene-1,4-diyl]bis[4-[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A



PAGE 1-B

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:1099063 CAPLUS Full-text

DOCUMENT NUMBER: 151:508432

TITLE: Hybrid Conjugated Organic Oligomers Consisting of Oligodiacetylene and Thiophene Units: Synthesis and Optical Properties

AUTHOR(S): Pilzrak, Gregor S.; van Grujthuisen, Kitty; van Doorn, Reinbert H.; van Lagen, Sander; Sudholter, Ernst J. R.; Zuilhof, Han

CORPORATE SOURCE: Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 6, Wageningen, 6703 HB, Neth. Chemistry—A European Journal (2009), 15(36), 9080-9096, S9085/1-S9085/19

CODEN: CHEUED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 151:508432

AB Novel and highly soluble hybrid conjugated organic oligomers consisting of oligodiacetylene and thiophene units have been synthesized in high purity through iterative and divergent approaches based on a sequence of Sonogashira reactions. The series of thiophene-containing oligodiacetylenes and homocoupled oligodiacetylenes show, both in solution and in the solid state, a strong optical absorption, which is progressively red shifted with increasing chain length. The linear correlation of the absorption maximum with the inverse of conjugation length (CL = number of double and triple bonds) shows that the effective conjugation length of this system is extended up to at least CL = 20. Furthermore, absorption measurements of dropcast thin films display not only a bathochromic shift of the absorption maxima but also a higher wavelength absorption, which is attributed to increased π - π interactions. The wavelength of the maximum fluorescence emission also increases with CL, and emission is maximal for oligomers with CL = 7-12 (fluorescence quantum yield Φ_F = .apprx.0.2). Both longer and shorter oligomers display marginal emission. The calculated Stokes shifts of these planar materials are relatively large (0.4 eV) for all oligomers, and likely due to excitation to the S2 state, thus suggesting that the presence of enyne moieties dominates the ordering of the lowest excited states. The fluorescence lifetimes (τ_F) are short (τ_{max} = 41 ns) and closely follow the tendency obtained for the fluorescence quantum yield. The anisotropy lifetimes show a near-linear increase with CL in line with highly rigid oligomers.

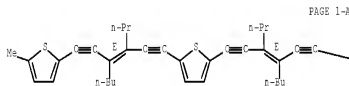
IT 1192820-75-EP 1122420-80-EP 1192820-84-EP
1192820-86-EP 1192820-90-EP 1192820-92-EP

RI: PREP (Properties); SPW (Synthetic preparation); PREP (Preparation) (synthesis via iterative Sonogashira coupling and optical properties of hybrid conjugated organic oligomers consisting of oligodiacetylene and thiophene units)

RN 1192820-75-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



PAGE 1-A

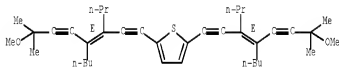


PAGE 1-B

RN 1192820-80-6 CAPLUS

CN Thiophene, 2,5-bis[(3E)-4-butyl-7-methoxy-7-methyl-3-propyl-3-octene-1,5-diyn-1-yl]- (CA INDEX NAME)

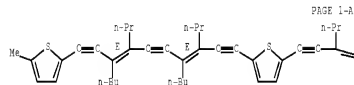
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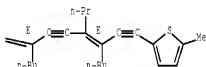
RN 1192820-84-0 CAPLUS

CN Thiophene, 2,5-bis[(3E,7E)-4-butyl-8-[2-(5-methyl-2-thienyl)ethynyl]ethynyl]-3,7-dipropyl-3,7-dodecadiene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

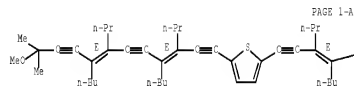


PAGE 1-B

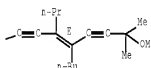
RN 1192820-86-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



PAGE 1-A

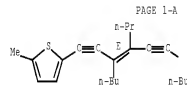


PAGE 1-B

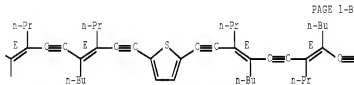
RN 1192820-90-8 CAPLUS

CN Thiophene, 2,5-bis[(3E,7E,11E)-4,8-dibutyl-12-[2-(5-methyl-2-thienyl)ethynyl]-3,7,11-tripropyl-3,7,11-hexadecatriene-1,5,9-triyn-1-yl]- (CA INDEX NAME)

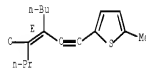
Double bond geometry as shown.



PAGE 1-A



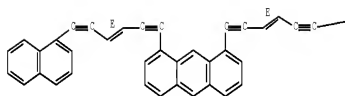
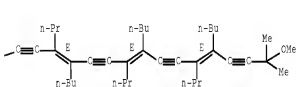
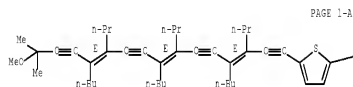
PAGE 1-B



PAGE 1-C

RN 1192820-92-0 CAPLUS

Double bond geometry as shown.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2007:46877 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 148:284829
 TITLE: Synthesis of smallest unit model of graphite
 intercalation compound and its possibility
 AUTHOR(S): Ogoshi, Senuke
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of
 Engineering, Osaka University, Japan
 SOURCE: Asahi Garasu Zaidan Josai Kenkyu Seika Hokoku (2006)
 01.03.07/1-01.03.07/8
 CODEN: AGSHEN; ISSN: 0919-9179
 PUBLISHER: Asahi Garasu Zaidan
 DOCUMENT TYPE: Journal; (computer optical disk)
 LANGUAGE: Japanese
 OTHER SOURCE(S): CASREACT 148:284829

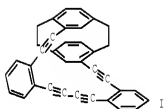
AB Graphite is perhaps the simplest layered structure. Many substances can be
 intercalated between layers of graphite. Upon intercalation, the graphite
 layers moved apart somewhat due to the intercalated atom. However, the layers
 still keep parallel each other which would be the key for the formation of
 intercalation compds. Thus, compds. having two aromatic rings, which can
 change the distance between the rings and keep parallel to each other, were
 designed and synthesized. The target compound was 1,8-bis[6-(1-naphthalenyl)-
 3-hexene-1,5-diynyl]anthracene.

IT 1007602-95-09
 RL: SPW (Synthetic preparation); PREP (Preparation)
 (preparation of bis[1(naphthalenyl)hexenediynyl]anthracene (smallest unit
 model for graphite intercalation compound))

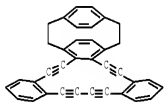
RN 1007602-95-0 CAPLUS
 CN Anthracene, 1,8-bis[(3E)-6-(1-naphthalenyl)-3-hexene-1,5-diyn-1-yl]- (CA
 INDEX NAME)

Double bond geometry as shown.

18 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2006:1027761 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 146:27609
 TITLE: Phane properties of
 [2.2]paracyclophane/dehydrobenzoannulene hybrids
 AUTHOR(S): Hlnrichs, Helno; Boydston, Andrew J.; Jones, Peter G.;
 Hess, Kirsten; Herges, Rainer; Haley, Michael M.;
 Hopt, Henning
 CORPORATE SOURCE: Institut fuer Organische Chemie, Technische
 Universitaet Braunschweig, Braunschweig, 38106,
 Germany
 SOURCE: Chemistry--A European Journal (2006), 12 (27),
 7103-7115
 CODEN: CHEUED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 146:27609
 GI



I



II

AB Macrocyclic hybrids of [2.2]paracyclophanes with dehydrobenzo[14]annulenes and dehydro[14]annulenes such as I and II are prepared. The UV/visible absorption spectra of the hybrids are compared to determine the communication between the aromatic rings of the paracyclophane units. For some of the title comps. and unsubstituted derivs., the anisotropy of induced c.d. is determined by calcn. to determine the effect of twisting in the perimeter of the macrocycles on the aromaticity of the component structures. The structures of a tetraethynyl[2.2]paracyclophane and of a twisted macrocyclic annulene are determined by X-ray crystallog.

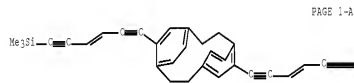
IT 375366-59-9E 865470-77-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and UV/visible absorption spectra of macrocyclic hybrids of [2.2]paracyclophanes with dehydrobenzo[14]annulenes and dehydro[14]annulenes and the anisotropy of induced c.d. and crystal structures of selected comps.)

RN 375366-59-9 CAPLUS

CN Tricyclo[8.2.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene, 5,11-bis[6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-, stereoisomer (CA INDEX NAME)



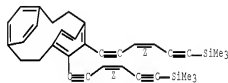
PAGE 1-A



PAGE 1-B

RN 865470-77-5 CAPLUS
CN Tricyclo[8.2.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene, 5,6-bis[6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



CS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yumiki

PATENT ASSIGNER(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIIXD2

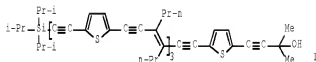
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

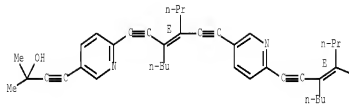
PATENT INFORMATION:

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WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
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RW: BW, GE, GM, KE, LS, MW, MZ, NA, SD, SI, SZ, TZ, UG, ZM, ZW, AG, AZ, BY, BG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, ML, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, NE, NG, SN, TD, TG				
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPL. INFO.: JP 2004-65446 A 20040309				
WO 2005-JP3950 W 20050308				
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT				
OTHER SOURCE(S): HARPAT 143:306181				
GI				

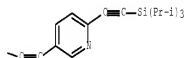


Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

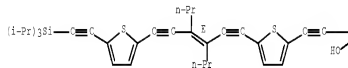


RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-([5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-([5-[(3E)-3-propyl-4-([5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound 1 was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-64-4D 740810-64-5D 740810-67-7B

740810-68-8D 864683-96-5D 864683-97-6D

864684-01-1D 864684-02-2D 864684-03-3D

864684-04-4D 864684-05-5D 864684-06-6D

RU: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

preparation); PREP (Preparation); RACT (Reactant or reagent)

(Intermediate; preparation of π -conjugated aromatic ring-containing acetylene

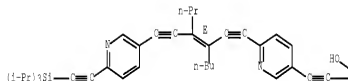
derivs. as organic electroluminescent devices)

RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

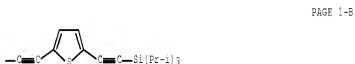
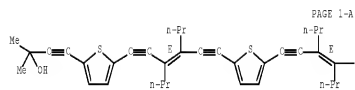


PAGE 1-B



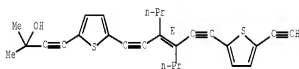
RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)



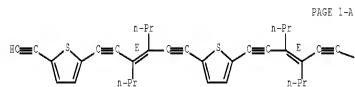
RN 864683-96-5 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-(2-(5-ethynyl-2-thienyl)ethynyl)-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



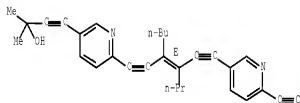
RN 864683-97-6 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-(2-[5-[(3E)-4-(2-(5-ethynyl-2-thienyl)ethynyl)-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



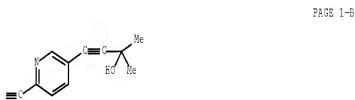
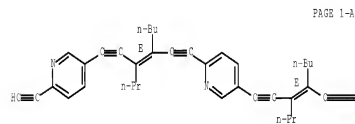
RN 864684-01-5 CAPLUS
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



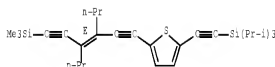
RN 864684-02-6 CAPLUS
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-04-8 CAPLUS
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

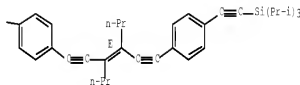
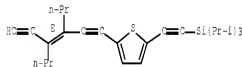


RN 864684-05-9 CAPLUS

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CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[(tris(1-methylethyl)silyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-31-1 CAPLUS

CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[(tris(1-methylethyl)silyl)ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[(tris(1-methylethyl)silyl)ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[(tris(1-methylethyl)silyl)ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

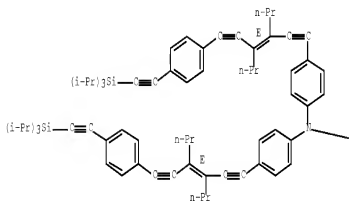
Double bond geometry as shown.

RN 864684-32-2 CAPLUS

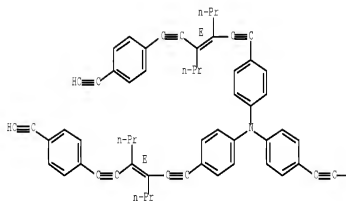
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

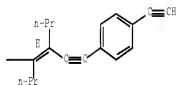
Double bond geometry as shown.

PAGE 1-A



PAGE 1-A

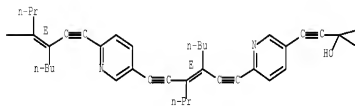
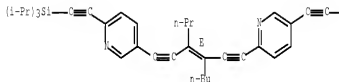




IT 740810-66-6P 740810-69-9P 864684-03-7P
 864684-06-7P 864684-09-1P 864684-21-3P
 864684-22-3P 864684-23-3P 864684-27-2P
 864684-28-3P 864684-29-4P 864684-29-5P
 864684-33-3P 864684-33-7P 864684-34-0P
 RL: DEV (Device component use); IMF (Industrial manufacture); SPN
 (Synthetic preparation); TEM (Technical or engineered material use); PREP
 (Preparation); USES (Uses)
 (preparation of π -conjugated aromatic ring-containing acetylene derivs. as
 organic electroluminescent devices)

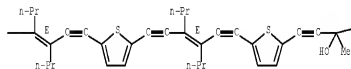
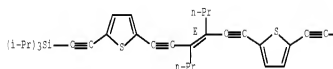
RN 740810-66-6 CAPLUS
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



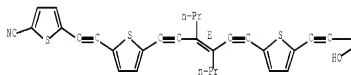
RN 740810-69-9 CAPLUS
 CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-pentan-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-pentan-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-03-7 CAPLUS
 CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-[3-hydroxy-3-methyl-1-butyn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-pentan-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

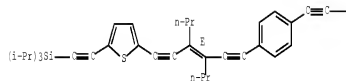
Double bond geometry as shown.



RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-(tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-(tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

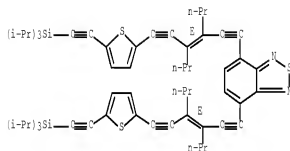
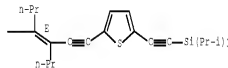
Double bond geometry as shown.



RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-(tris(1-methylethyl)silyl]ethynyl)-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

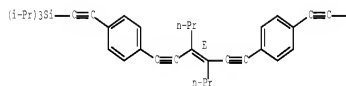
Double bond geometry as shown.



RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

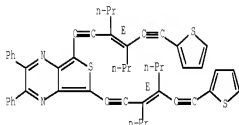
Double bond geometry as shown.

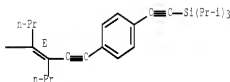


RN 864684-09-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

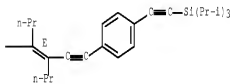
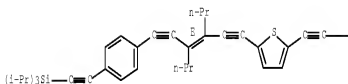




RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

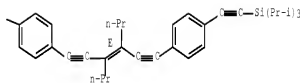
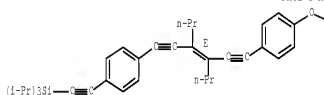
Double bond geometry as shown.



RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diene-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis(tris(1-methylethyl)- (9CI) (CA INDEX NAME)

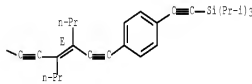
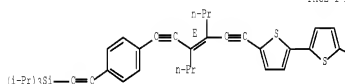
Double bond geometry as shown.



RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

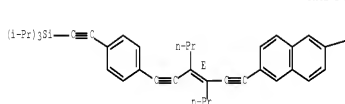
Double bond geometry as shown.

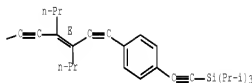


RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[[3E]-3,4-dipropyl-6-[4-[2-(tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diy-1-yl]-6-[[3E]-3-propyl-4-[2-[4-[2-(tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

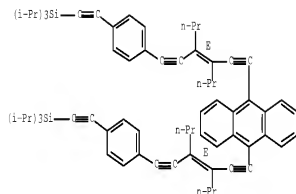




RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-1-yl]- (CA INDEX NAME)

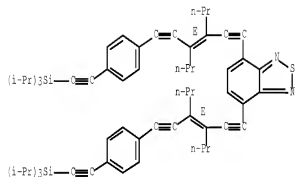
Double bond geometry as shown.



RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-1-yl]- (CA INDEX NAME)

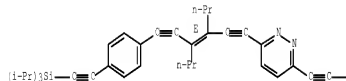
Double bond geometry as shown.



RN 864684-29-7 CAPLUS

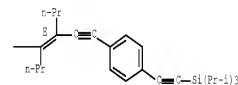
CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

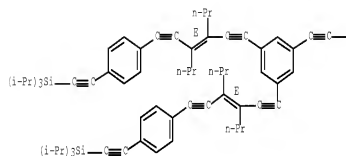
PAGE 1-B



RN 864684-30-0 CAPLUS

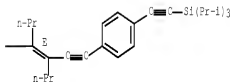
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

PAGE 1-B

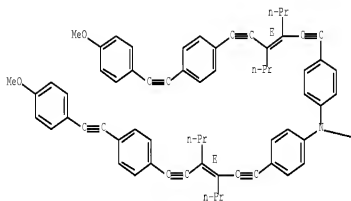


RN 864684-33-3 CAPLUS

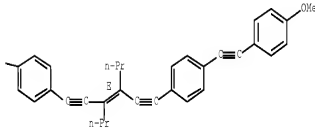
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

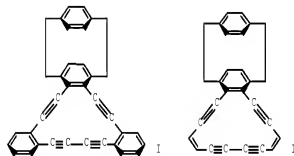


PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

18 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2005:630411 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 143:346727
 TITLE: [2.2]Paracyclophane/Dehydroannulene Hybrids: Probing the Aromaticity of the Dehydro[14]annulene Framework
 AUTHOR(S): Hinrichs, Helmut; Fischer, Axel W.; Jones, Peter G.; Hopf, Henning; Haley, Michael M.
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA
 SOURCE: Organic Letters (2005), 7(17), 3793-3795
 CODEN: ORLEF7; ISSN: 1523-7050
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:346727
 GI



AB The synthesis of [2.2]paracyclophane/dehydro[14]annulene hybrids I and II is reported. Comparison of the proton NMR spectra of I and II with their open precursors and with related model compds. reveals the pronounced effect of macrocycle formation upon the cyclophane protons H15/H16, which lie above the shielding cone of the diatropic [14]annulene moiety.

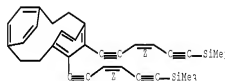
II 865470-27-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (paracyclophane dehydroannulene hybrids probing aromaticity of dehydroannulene framework)

RN 865470-27-5 CAPLUS

CN Tricyclo[6.2.2.2(4,7)]hexadeca-4,6,10,12,13,15-hexaene, 5,6-bis[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2005:394187 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:333

TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(2)-hexen-1,5-diyne, 2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their derivatives

AUTHOR(S): Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung

CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan

SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575

CODEN: BMCEP; ISSN: 0968-0896

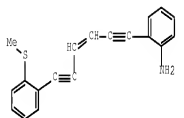
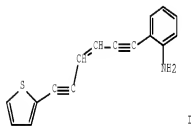
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:333

GI



AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from <0.01 to 96.6 μ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10⁻⁷M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(2)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between

the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 85C419-13-7P

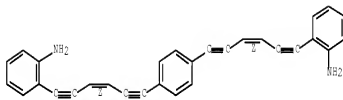
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOD (Biological study); PREP (Preparation)

(cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(2)-hexen-1,5-diyne, 2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their derivs.)

RM 85C619-13-7 CAPLUS

CN Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2005:17022 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:113747

TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents

INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong

PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan

SOURCE: U.S. Pat. Appl. Publ., 41 pp.

CODEN: USXXXX

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050004212	A1	20050106	US 2004-847667	20040518
US 7332623	B2	20080219		
CA 2570366	A1	20050317	CA 2004-2570366	20040909
WO 2005023131	A2	20050317	WO 2004-US29334	20040909
WO 2005023131	A3	20050512		

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													US 2003-483887P	P 20030630	
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CN 1842306	A	20061004	CN 2004-80024581	20040909											
CN 1842307	A	20061004	CN 2004-80024602	20040909											
BR 2004013534	A	20061010	BR 2004-13534	20040909											
BR 2004014232	A	20061031	BR 2004-14232	20040909											
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LUSIS DISCOVERY FORMAT OTHER SOURCE(S): MARPAT 142-113747															

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LISTS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 142:113747

CI



Q=



Q1=



I

AB This invention provides aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts or solvates thereof (wherein: R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxymethyl, tetrahydropyranyloxycarbonyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). These compds. found to have inhibitory activities against topoisomerase I or act as a S phase or G2/M phase blocker and were also tested in vitro in anticancer assay. 4-((Z)-3-dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

IT 457914-65-7P

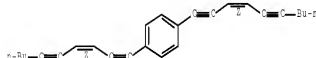
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOD (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)

RN 457914-65-7 CAPLUS

CH Benzene, 1,4-di((3Z)-3-decenen-1,5-diyn-1-yl)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:15944 CAPLUS [Full-Text](#)

DOCUMENT NUMBER: 142:113746

TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents and pharmaceutical compositions comprising them

INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong

PATENT ASSIGNER(S): Kachung Medical University, Taiwan

SOURCE: U.S. Pat. Appl. Publ., 41 pp.

CODEN: USKXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050004211	A1	20050106	US 2004-847659	20040518
CA 2570366	A1	20050317	CA 2004-2570366	20040909
WO 2005023131	A2	20050317	WO 2004-US293334	20040909
WO 2005023131	A3	20050512		
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WO 2005023143	A2	20050317	WO 2004-US293335	20040909
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WO 2005023144	A3	20050512		
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WO 2005023145	A3	20050512		
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WO 2004-US293336 W 20040909
WO 2004-US293337 W 20040909
WO 2004-US293338 W 20040909
US 2006-488204 A1 20060718

OTHER SOURCE(S): MARPAT 142:113746

GI



Q=



Q1=



AB A pharmaceutical compns. comprises aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxyethyl, tetrahydropyranyloxypropyl or Ph when R1 = R2 = H and R4 = o-cynophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). The pharmaceutical composition is used to treat a subject afflicted with a tumor/cancer by inhibiting topoisomerase I activities or blocking the S phase or G2/M phase of the tumor/cancer cells. The tumor/cancer cell is selected from leukemia cancer cells, non-small-cell lung cancer cells, col on cancer cells, CNS cancer cells, melanoma cancer cells, ovarian cancer cells, renal cancer cells, prostate cancer cells and breast cancer cells. These compds. were tested in vitro for inhibitory activities against topoisomerase I, cell cycle at a S phase or G2/M phase blocker, and anticancer growth. For example, 4-((Z)-3-Dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor K562 cells.

IT

457914-63-7P

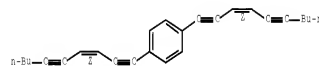
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOI (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)

RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

PRIORITY APPLN. INFO.:

US 2003-463887P P 20030630
US 2003-501266P P 20030930
US 2004-832168 A 20040426
US 2004-842302 A 20040510
US 2004-847429 A 20040517
US 2004-887644 A 20040709
US 2004-887667 A 20040709
US 2004-888206 A 20040709
JP 2006-524963 A3 20040909
JP 2006-524964 A3 20040909
RU 2006-106621 A3 20040909
WO 2004-US293334 W 20040909
WO 2004-US293335 W 20040909

L8 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:480115 CAPLUS Full-text

DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Eneidyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

PAGE 1-B

AUTHOR(S): Nakano, Yuki; Ishizuka, Kenichi; Muraoka, Kenji;

Ohtani, Hiroyuki; Takayama, Yuki; Sato, Fumio

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

SOURCE: Organic Letters (2004), 6(14), 2373-2376

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

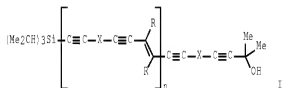
GI



RN 740810-62-2 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-([4-[(3E)-3-propyl-4-([4-[(3E)-3-propyl-4-([4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hepten-1-yn-1-yl]phenyl)- (CA INDEX NAME)

Double bond geometry as shown.



AB Synthesis and fluorescence properties of π -conjugated compds. I ($n = 1-3$; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroarom. ring and an eneidyne unit in the backbone are described.

IT 740810-61-1P 740810-62-2P 740810-64-4P

740810-63-5P 740810-67-7P 740810-68-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PRGP (Preparation); RACT (Reactant or reagent)

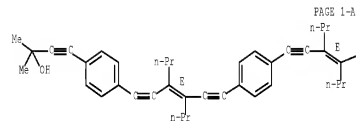
(preparation and absorption and fluorescence spectra of conjugated oligomers

having aromatic (or heteroarom.) and eneidyne units alternately in the backbone)

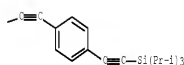
RN 740810-61-1 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-([4-[(3E)-3-propyl-4-[2-([4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



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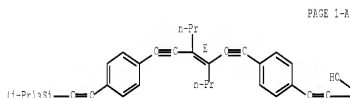


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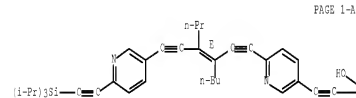
RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



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PAGE 1-A

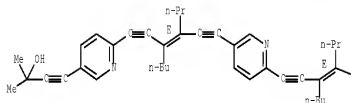


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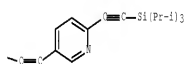
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

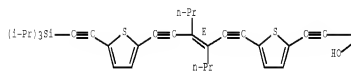


RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

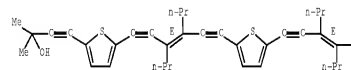


RN 740810-69-8 CAPLUS

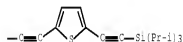
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



IT 740810-63-3P 740810-64-4P 740810-63-3P

RL: PFP (Properties); SEM (Synthetic preparation); PREP (Preparation)
(preparation and absorption and fluorescence spectra of conjugated oligomers

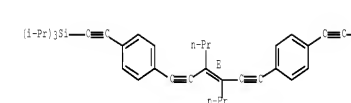
having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

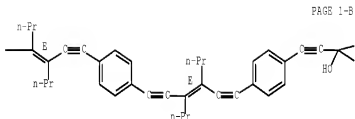
RN 740810-63-3 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A





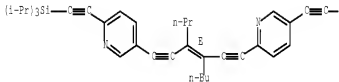
PAGE 1-C



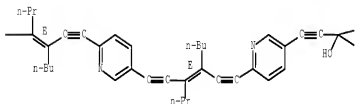
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CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



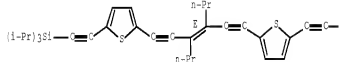
PAGE 1-C



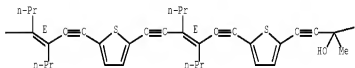
RN 740810-69-9 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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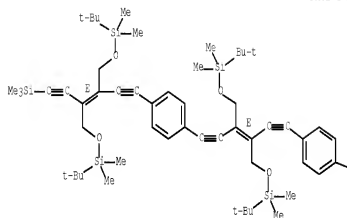
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REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

18 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:328526 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 141:54000
TITLE: Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylacetacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions
AUTHOR(S): Utesch, Wils F.; Diederich, Francois; Boudon, Corinne; Glsselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg,
 HCI, Zurich, CH-8093, Switz.
 SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718
 CODEN: HCACAV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:54000

PAGE 1-A

AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodophenyl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-1[CH4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 (I, n = 2-4) a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I (n = 1-4) shift bathochromically with increasing oligomeric length, from λ_{max} 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π -Electron conjugation in these oligomers is less efficient than in



PAGE 1-B

Me3Si[CH4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 (II) due to poor transmittance of π -electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield $\Phi_F = 0.69$ measured for I (n = 3). Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

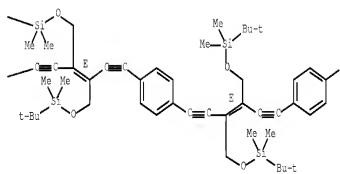
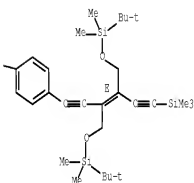
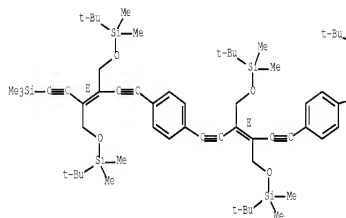
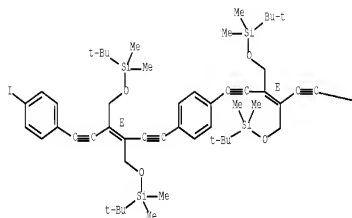
IT 554459-61-UP 554459-62-UP 554459-64-UP
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (solid-phase synthesis of oligo(triacetylene)s and
 oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz
 cross-coupling reactions)

RN 554459-62-0 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-([4-[(3E)-6-(4-iodophenyl)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

RN 554459-63-1 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-([4-[(3E)-6-(4-iodophenyl)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.



RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

II 704916-29-0P

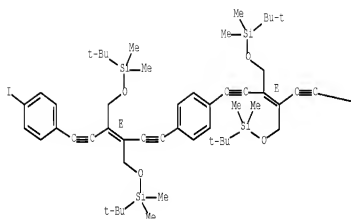
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadot-Chodkiewicz cross-coupling reactions)

RN 704916-29-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[[4-(iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

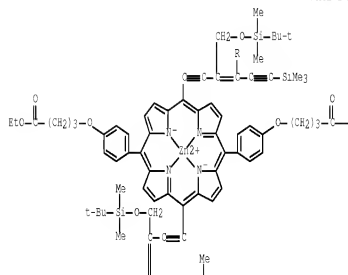


PAGE 1-B



dimethyl[ethyldimethylsilyloxy]methyl)-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl-
 x[21],x[22],x[23],x[24]bis(4,1-phenylacetoxy)]bis[butanato]](2-)-, (SP-4-1)- (3CI) (CA INDEX NAME)

PAGE 1-A



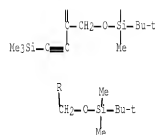
PAGE 1-B

OS.CITING REF COUNT: 6 THERE ARE 6 CAPIUS RECORDS THAT CITE THIS RECORD
 (6 CITINGS)
 REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 39 CAPIUS COPYRIGHT 2009 ACS ON STM
 ACCESSION NUMBER: 2003:1000504 CAPIUS [Full-text](#)
 DOCUMENT NUMBER: 141:242819
 TITLE: Product class 4: organometallic complexes of copper
 AUTHOR(S): Heaney, E.; Christie, S.
 CORPORATE SOURCE: Dept. of Chemistry, University of Loughborough,
 Loughborough, LE11 3TU, UK
 SOURCE: Science of Synthesis (2004), 3, 305-662
 CODEN: SSCUJ9
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English
 AB A review. The use of copper and related complexes in applications to organic
 synthesis is reviewed.
 IT 219463-15-5P 375366-59-9P
 RL: SPH (Synthetic preparation); PREP (Preparation)
 (applications of copper and organocopper complexes to organic synthesis)
 RN 219463-15-5 CAPIUS
 CN Zinc, [[diethyl 4,4'-[[10,20-bis[(3E)-3,4-bis[[[1,1-

-OEt

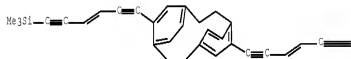
PAGE 2-A



RN 375366-59-9 CAPIUS
 CN Tricyclo[8.2.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene,

5,11-bis[6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-, stereoisomer (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 1706 THERE ARE 1706 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2003:592887 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 140120929
TITLE: Third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores
AUTHOR(S): Concilio, S.; Biaggio, I.; Gunter, P.; Plotto, S. P.; Edelmann, M. J.; Raimundo, J.-M.; Diederich, F.
CORPORATE SOURCE: Swiss Federal Institute of Technology, Institute of Quantum Electronics, Nonlinear Optics Laboratory, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Journal of the Optical Society of America B: Optical Physics (2003), 20 (8), 1656-1660
CODEN: JOBPCE; ISSN: 0740-3224
PUBLISHER: Optical Society of America
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new approach to tuning the nonlinear optical properties of hybrid oligo(triacetylene) compds. was studied. The method is based on the insertion of a central heterospacer group between two (E)-hex-3-ene-1,5-diyne moieties. A significant increase in the 2nd hyperpolarizability γ is expected if the central spacer fragment is an extended conjugated chromophore. The authors present mols. with enhanced 2nd hyperpolarizability caused by the presence of highly conjugated spacer groups, which increase the overall π -electron delocalization. Some metal complexes obtained from the coordination of these hybrid oligomers to transition-metal centers also were studied and revealed substantial differences in the capacities of the metal centers to act as electronic bridges. Finally, theor. predictions of the relative differences in the 2nd hyperpolarizabilities of the new spacer compds. are in good agreement with the exptl. results.

IT 628738-17-A 628738-18-1 628738-19-2

628738-20-6

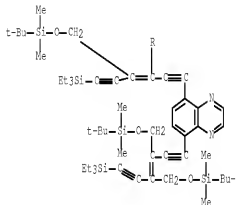
RI: PRP (Properties)

(third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores)

RN 628738-17-0 CAPLUS

CN Quinoxaline, 5,8-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxymethyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]- (9CT) (CA INDEX NAME)

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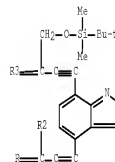
PAGE 2-A



RN 628738-18-1 CAPLUS

CN 2,1,3-Benzoxadiazole, 4,7-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxymethyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

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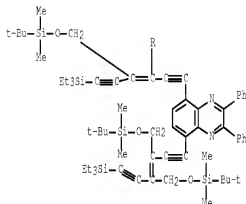
PAGE 3-A



RN 628738-19-2 CAPLUS

CN Quinoxaline, 5,8-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl- (CA INDEX NAME)

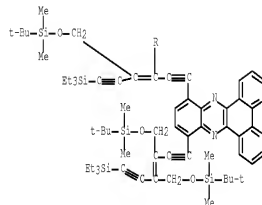
PAGE 1-A



RN 628738-20-5 CAPLUS

CN Dipyrro[3,2-a:2',3'-c]phenazine, 10,13-bis[3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (3CI) (CA INDEX NAME)

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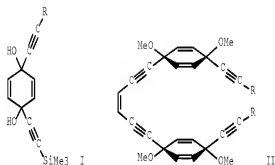
PAGE 2-A



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
 REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

18 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2009 ACS on SIN
 ACCESSION NUMBER: 2003:491916 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 139:395637

TITLE: Synthesis of differentially protected/functionalised acetylenic building blocks from p-benzoquinone and their use in the synthesis of new enediyne
 AUTHOR(S): Sankararaman, Sethuraman; Srinivassan, Manivannan
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology Madras, Madras, 600 036, India
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(13), 2388-2392



AB Sequential addition of two different lithium acetylides to p-benzoquinone yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4-diols I [R = (Me₂CH)SSi, (EtO)2CH] with different protective/functional groups on the two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to the corresponding terminal acetylides followed by Pd(0)-mediated coupling with (E)-1,2-dichloroethane yielded new enediyne II bearing cyclohexa-2,5-diene units.

IT 626235-22-99
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of cyclohexadienyl enedynes via double addition of functionalized

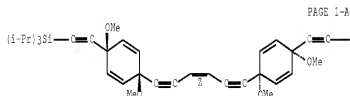
lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethane)

RN 626235-20-9 CAPLUS

CN Silane, [(3E)-3-hexene-1,5-diyne-1,6-diylbis[(cis-1,4-dimethoxy-2,5-cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



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-Si(Pr-i)₃

IT 626235-21-99 626235-22-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cyclohexadienyl enedynes via double addition of functionalized

lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethane)

RN 626235-21-0 CAPLUS

CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-(3,3-dimethoxy-1-propynyl)-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



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-OEt

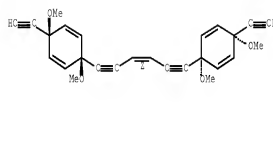
PAGE 1-B

RN 626235-22-1 CAPLUS

CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-ethynyl-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



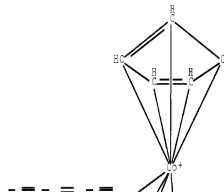
OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS APPEAR IN THE RE FORMAT

18 ANSWER 15 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2003:345601 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 139:149735
 TITLE: Butterfly topologies: new expanded carbon-rich organometallic scaffolds
 AUTHOR(S): laskoski, Matthew; Roidl, Gaby; Ricks, Holly L.; Morton, Jason G. M.; Smith, Mark D.; Bunz, Uwe H. F.
 CORPORATE SOURCE: USC NanoCenter, Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC, 29208, USA
 SOURCE: Journal of Organometallic Chemistry (2003), 673 (1-2), 13-24
 CODEN: JORCAL; ISSN: 0022-328X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:149735
 GI

PAGE 1-A



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

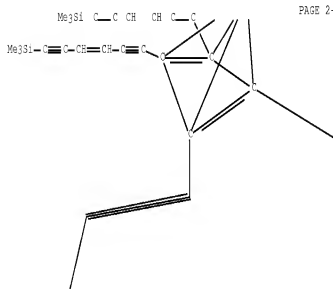
AB Starting from either (tetraethynylcyclobutadiene)cyclopentadienylcobalt or [1,2-diethynyl-3,4-(2-dioxanylcyclobutadiene)cyclopentadienylcobalt a sequence of copper and Pd-catalyzed couplings of the Eglinton and Heck-Cassar-Sonogashira-Hagihara type furnished five bow-tie shaped doubly annelated dehydroannulenes, the largest of which featured a (formal) 7,8:13,14:23,26:31,32-tetra(4'-alkyl-1'',2''-benzo)tricyclo[18,16,02,19]hexatricosa-3,5,9,11,15,17,21,23,27,29,33,35-dodecayne-1,7,13,19,25,31-hexaene hydrocarbon ligand with a cyclopentadienylcobalt-stabilized cyclobutadiene complex as its central unit (I) (R = i-Pr, n-Bu). Single crystal X-ray structures of two of the smaller butterflyfiles (II) and (III) are reported and their surprising solid-state packing is discussed herein. The solid state structure of III was also examined via PM3 calcons.

II 349453-20-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PRSP (Preparation); RACT (Reactant or reagent)
 (preparation, crystal structure, and PM3 calcon. of butterfly dehydro[14]annulenes and dehydro[18]annulenes containing a cyclobutadiene(cyclopentadienyl)cobalt unit)

RN 349453-20-9 CAPLUS

CN Cobalt, (η⁵-2,4-cyclopentadien-1-yl)[{[(1,2,2a,18a-η)-3,4,8,10,11,12,17,18-octadehydro-7,14-bis(1,1-dimethylethyl)dibenzo[a,1]cyclobuta[e]cyclootetradecene-1,2-diyl]di-(3z)-hexene-1,5-diyne-6,1-diyl]bis(trimethylsilane)]- (9CI) (CA INDEX NAME)



PAGE 2-A

TITLE: Acetylenic scaffolding on solid support:
Poly(triacetylene)-derived oligomers by Sonogashira
and Cadot-Chodkiewicz-type cross-coupling reactions

AUTHOR(S): Utesch, Nils F.; Diederich, Francois

CORPORATE SOURCE: Laboratorium für Organische Chemie, ETH-Honggerberg,
HCI, Zurich, CH-8093, Switz.

SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239
CODEN: OBGMK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:85055

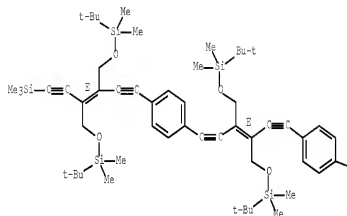
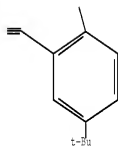
AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., 1[4-(CH4C.tplbond.CCR:CCR.tplbond.C)nSiMe3 (R = CH2OSiBocMe2, n = 1, 2, 3, 4)] members of a new class of linearly π -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

IT 554453-82-20 554453-67-10 554453-64-20
RI: PREP (Properties); SYN (Synthetic preparation); PREP (Preparation) (electronic absorption and emission, UV/VIS spectra);
poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)

RN 554453-62-0 CAPLUS

CN 4,9-Dioxo-3,10-disiladodeca-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

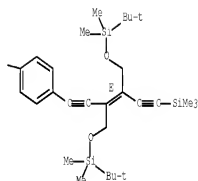
Double bond geometry as shown.



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2003:234291 CAPLUS Full-text
DOCUMENT NUMBER: 139:85055

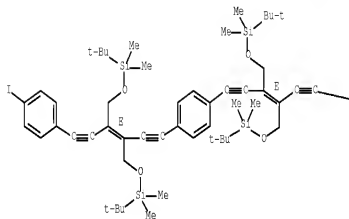


RN 554459-63-1 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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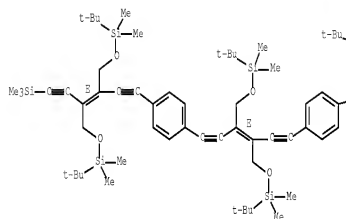


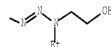
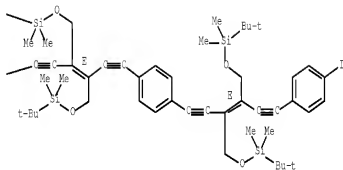
RN 554459-64-2 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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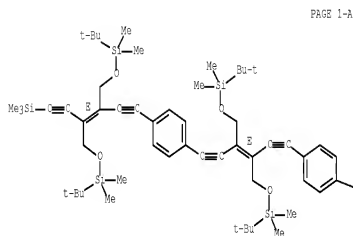
IT 554459-71-106, Merrifield resin-supported
 554459-70-106, Merrifield resin-supported 554459-70-106
 , Merrifield resin-supported
 RL: RCT (Reactant); SPN (Synthetic preparation); PRFP (Preparation); RACT
 (Reactant or reagent)

(preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed
 cross-coupling reactions of supported poly(triacetylene)-derived
 oligomers)

RN 554459-71-1 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

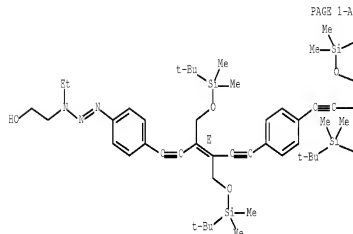


PAGE 1-A

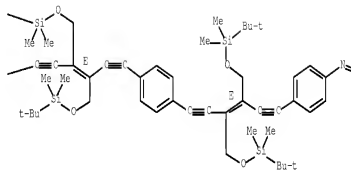
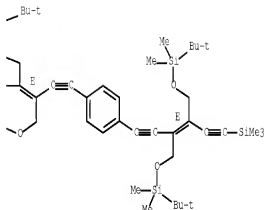
RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.



PAGE 1-A

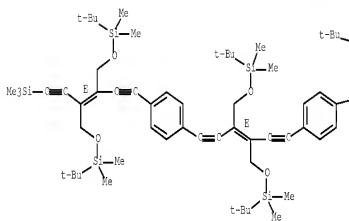


RN 554459-73-3 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

PAGE 1-C

Double bond geometry as described by E or Z.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)
 REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

18 ANSWER 17 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2002:874017 CAPLUS Full-text
 DOCUMENT NUMBER: 138:72938
 TITLE: Diatropicity of 3,4,7,8,9,10,13,14-Octadehydro[14]annulenes: A Combined Experimental and Theoretical Investigation
 AUTHOR(S): Boydston, Andrew J.; Haley, Michael M.; Williams, Richard Vaughan; Armantrout, John R.
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA
 SOURCE: Journal of Organic Chemistry (2002), 67(25), 8812-8819
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:72938
 AB The synthesis and study of a series of octadehydro[14]annulenes is described. The aromaticity of these annulenes was investigated through examination of exptl. data from arene-fused systems as well as calculated nucleus-independent chemical shifts (NICS) and bond lengths. Benzene ring fusion to the parent system results in a stepwise loss in aromaticity as the number of fused rings is increased from one to two to three. This decrease in annulenic ring current is manifested in the alkene proton chemical shifts (0-2 benzenes) as well as the NICS (0-3 benzenes). Comparison of isomeric thiophene-fused

annulenes shows further evidence of ring current competition as these allow for observation of intermittent degrees of delocalization throughout the annulenic core. A consistent relationship between the magnitude of the NICS values and the degree of benzannulation is also observed

IT 482294-11-3P

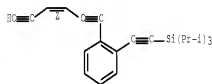
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cross-coupling; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482294-19-9 CAPLUS

CN Benzene, 1-((3E)-3-hexene-1,5-diyn-1-yl)-2-((tris(1-methylethyl)silyl)ethynyl)- (CA INDEX NAME)

Double bond geometry as shown.



IT 482294-11-7P 482294-20-2P 482294-21-3P

482294-22-4P

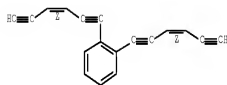
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cyclization; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482294-17-7 CAPLUS

CN Benzene, 1,2-di((3E)-3-hexene-1,5-diyn-1-yl)- (CA INDEX NAME)

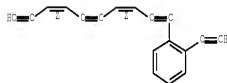
Double bond geometry as shown.



RN 482294-20-2 CAPLUS

CN Benzene, 1-((3E,7E)-3,7-decadiene-1,5,9-triyn-1-yl)-2-ethynyl- (CA INDEX NAME)

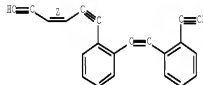
Double bond geometry as shown.



RN 482294-21-3 CAPLUS

CN Benzene, 1-ethynyl-2-[[2-((3E)-3-hexene-1,5-diynyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

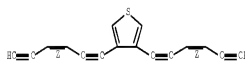
Double bond geometry as shown.



RN 482294-22-4 CAPLUS

CN Thiophene, 3,4-di((3E)-3-hexene-1,5-diyn-1-yl)- (CA INDEX NAME)

Double bond geometry as shown.



IT 482294-15-5P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection/cyclization; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482294-15-5 CAPLUS

CN Thiophene, 2,3-bis((3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl)- (CA INDEX NAME)

Double bond geometry as shown.



IT 381173-15-5P 381173-16-1P 482294-13-7P

482294-14-4P

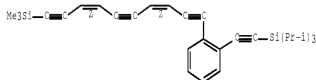
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 381173-15-5 CAPLUS

CN Benzene, 1-((3E,7E)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl)-2-((2-(tris(1-methylethyl)silyl)ethynyl)- (CA INDEX NAME)

Double bond geometry as shown.



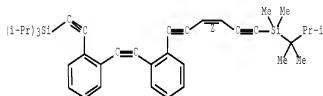
PAGE 1-8

—Si(Pr-1)3

RN 381173-20-2 CAPLUS

CN Silane, [[2-[[2-[(3Z)-6-(dimethyl(1,1,2-trimethylpropyl)silyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]phenyl]ethynyl]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

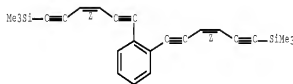
Double bond geometry as shown.



RN 482294-13-3 CAPLUS

CN Silane, [1,2-phenylenedi-[(3Z)-3-hexene-1,5-diyn-6,1-diyl]bis(trimethyl- (9CI) (CA INDEX NAME)

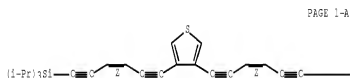
Double bond geometry as shown.



RN 482294-14-4 CAPLUS

CN Thiophene, 3,4-bis[[3Z)-6-[tris(1-methylethyl)silyl]-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

IT 36)75-15-5P

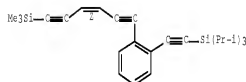
RL: RCT (Reactant); SEN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection; a combined expl. and theor. investigation of diastereotropy of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 381173-13-3 CAPLUS

CN Benzene, 1-[[3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (33 CITINGS)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2002:874016 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:72902

TITLE: Dimethyldihydropropyne-Dehydrobenzoannulene Hybrids: Studies in Aromaticity and Photoisomerization

AUTHOR(S): Kimball, David B.; Haley, Michael M.; Mitchell, Reginald H.; Ward, Timothy R.; Bandyopadhyay, Subhasjit; Williams, Richard Vaughan; Armantrout, John R.

CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Journal of Organic Chemistry (2002), 67(25), 8798-8811
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:72902

AB The synthesis and study of dehydrobenzoannulene (DBA)-dimethyldihydropropyne (DDP) hybrids as models for the investigation of aromaticity in weakly diastropic systems is reported. Three new monofused DBA-DDP hybrids have been synthesized, and their NMR spectra are discussed with regard to quantifying the aromaticity remaining in multibenzene-fused DBAs. Nucleus-independent chemical shifts, determined at a series of locations for each compound, bond lengths, and 1H and 13C NMR chemical shifts were calculated and used to probe

the aromaticity of these hybrids. Systems where more than one annulene/CBA is fused to the DCP core have also been obtained, and their potential use in photoinduced isomerization applications is discussed.

IT 481713-23-5f

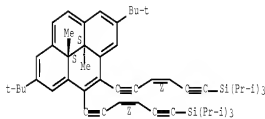
RU: RCT (Reactant); SPN (Synthetic preparation); PRDP (Preparation); RACT (Reactant or reagent)

(desilylation/cyclization; studies in aromaticity and photoisomerization of dimethyldihydropyrene-dehydrobenzoannulene hybrids)

RN 481713-23-5 CAPLUS

CN Pyrene, 2,7-bis(1,1-dimethylethyl)-10h,10c-dihydro-10h,10c-dimethyl-4,5-bis(32)-6-[tris(1-methylethyl)silyl]-3-hexene-1,5-diyn-1-yl]-, (10h,10c)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)

REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2002:719354 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:25161

TITLE: Third-order nonlinear optical properties of in-backbone substituted conjugated polymers

AUTHOR(S): Gubler, U.; Concello, S.; Bosshard, Ch.; Blagpio, I.; Gunter, P.; Martin, R. E.; Boelmann, M. J.; Wytko, J. A.; Clederich, F.

CORPORATE SOURCE: Institute of Quantum Electronics, ETH-Honggerberg, Zurich, CH-8093, Switz.

SOURCE: Applied Physics Letters (2002), 81(13), 2322-2324

COCEN: APPLAB; ISSN: 0003-6951

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An alternative approach for tuning of the third-order nonlinear optical properties of organic mols. is based on insertion a functional group into the path of the π -electron conjugation instead of at chain ends. This scheme enhances the second-order hyperpolarizability for short mols., but in two instances where such mols. were polymerized into longer mols. the overall hyperpolarizability was lower. The study is based on tert-butyl(dimethylsilyloxy)-vinyl-poly(triacetylene) as the basic linear conjugated polymer, with spacer of anthracene, benzene, naphthalene, thiophene, tetramethylbenzene, furan tetrafluorobenzene, pyridine, biphenyl, pyrazine, and bis(triethylphosphine-Pt).

IT 249616-79-3 249616-82-8,

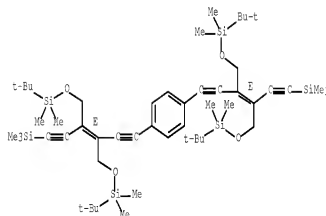
2,6-Bis[(E)-3,4-bis[[tert-butyl(dimethylsilyloxy)methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]naphthalene 249616-33-3,
9,10-Bis[(E)-3,4-bis[[tert-butyl(dimethylsilyloxy)methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]anthracene 249616-84-8
249616-87-3, 1,4-Bis[(E)-3,4-bis[[tert-butyl(dimethylsilyloxy)methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene 249616-88-4 249616-89-5
2,5-Bis[(E)-3,4-bis[[tert-butyl(dimethylsilyloxy)methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]pyrazine 249616-90-8
249616-91-3, 2,5-Bis[(E)-3,4-bis[[tert-butyl(dimethylsilyloxy)methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]furan
RU: PRP (Properties)

(role of in-backbone spacer on third-order nonlinear optical properties of polyacetylene conjugated polymers)

RN 249616-79-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octanethy-7-[[trimethylsilyl]ethynyl]-, (6E,6'E)-(SC1) (CA INDEX NAME)

Double bond geometry as shown.

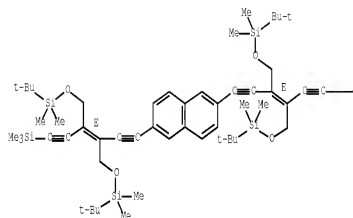


RN 249616-82-8 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,6-naphthalenediyl-di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octanethy-7-[[trimethylsilyl]ethynyl]-, (6E,6'E)-(SC1) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



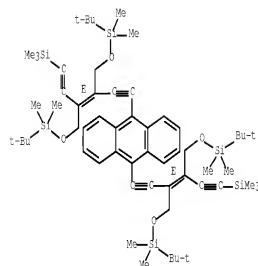
PAGE 1-B

—SiMe₃

RN 249616-83-9 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(9,10-anthracenediyl)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (3CI) (CA INDEX NAME)

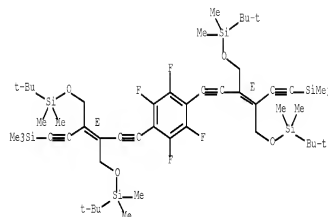
Double bond geometry as shown.



RN 249616-84-0 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (3CI) (CA INDEX NAME)

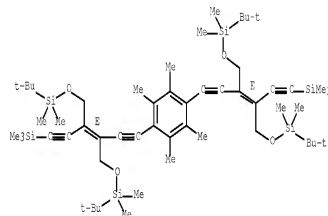
Double bond geometry as shown.



RN 249616-87-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (3CI) (CA INDEX NAME)

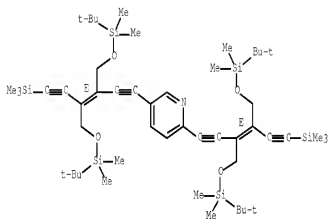
Double bond geometry as shown.



RN 249616-88-4 CAPLUS

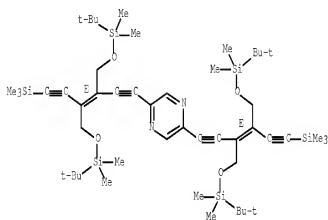
CN Pyridine, 2,5-bis[[3E]-3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxymethyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



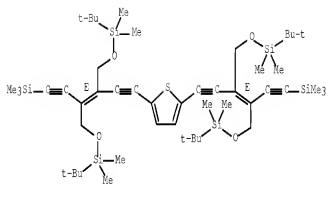
RN 249616-89-5 CAPLUS
 CN Pyrazine, 2,5-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-dien-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



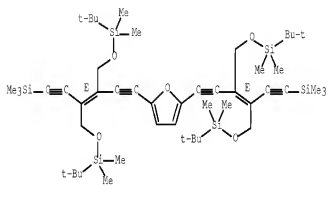
RN 249616-90-8 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,5-thiophenediyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (SCI) (CA INDEX NAME)

Double bond geometry as shown.



RN 249616-91-9 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,5-furandiyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (SCI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
 REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2002:700080 CAPLUS Full-text
 DOCUMENT NUMBER: 138:247934
 TITLE: Cytotoxicities and topoisomerase I inhibitory activities of 2-(2-(2-alkynylphenyl)ethynyl)benzonitriles, 1-aryldec-3-ene-1,5-diones, and related bis(enediynyl)arene compounds
 AUTHOR(S): Lin, Chi-Fong; Lu, Wen-Dar; Hsieh, Pei-Chen; Kuo, Yao-Haur; Chiu, Huey-Fen; Wang, Chyi-Jia; Wu, Ming-Jung
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan
 SOURCE: Helvetica Chimica Acta (2002), 85(8), 2564-2575
 CODEN: HCAQNV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:247934

AB The activities of a series of acyclic enediyne, 2-(6-substituted hex-3-ene-1,5-diynyl)benzotrifurans (1-5) and their derivs. 7-23 were evaluated against several solid tumor cell lines and topoisomerase I. Comps. 1-5 show selective cytotoxicity with Hepa cells, and 2-(6-phenylhex-3-ene-1,5-diynyl)benzotrifurans (5) reveals the most-potent activity. Analogs 8-10 and 13-23 also have the same effect with DLD cells; 1-[(2)-dec-3-ene-1,5-diynyl]-4-nitrobenzene (21) shows the highest activity among them. Moreover, 1-[(12)-dec-3-ene-1,5-diynyl]-2- (trifluoromethyl)benzene (20) exhibits the strongest inhibitory activity with the HeLa cell line. Derivs. 9, 10, 18, and 23 display inhibitory activities with topoisomerase I at 87 μ M. The cell-cycle anal. of compound 5, which induces a significant blockage in S phase, indicates that these novel enediyne probably undergo other biol. pathways leading to the cytotoxicity, except the inhibitory activity toward topoisomerase I.

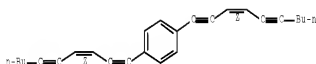
IT 457934-65-74

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cytotoxicity and topoisomerase I inhibitory activity of
2-[2-(2-alkynylphenyl)ethynyl]benzotrifurans,
1-aryldec-3-ene-1,5-diyne, and related bis(enediynyl)arene compds.)

RN 457934-65-7 CAPLUS

CN Benzene, 1,4-di[(3)-3-dec-ene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2002:628032 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:4578

TITLE: Dramatically enhanced fluorescence of heteroaromatic chromophores upon insertion as spacers into

oligo(triacetylene)s
Edelmann, Michael J.; Raimundo, Jean-Manuel; Utesch, Nils F.; Diederich, Francois

CORPORATE SOURCE: Lab. Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.

SOURCE: Helvetica Chimica Acta (2002), 85(7), 2195-2213

CODEN: HCACNV; ISSN: 0018-019X

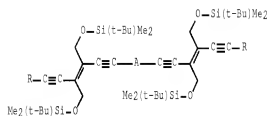
PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:4578

GI



I

AB In continuation of a previous study on the modulation of π -electron conjugation of oligo(triacetylene)s by insertion of central hetero-spacer fragments between two (E)-hex-3-ene-1,3-diyne ((E)-1,2-diethynylbenzene, DEE) moieties, trimeric hybrid oligomers (1; A = spacer, R = SiEt3, SiMe3) were prepared. Spacers used were both electron-deficient (quinacoline-based heterocycles, pyridazine) and electron-rich (2,2'-bithiophene, 5,3-dioctyl-9H-fluorene)chromophores. With a dipyrrolophenazine spacer, transition metal complexes were synthesized as potential precursors for nanoscale scaffolding based on both covalent acetylenic coupling and supramol. assembly. The UV/visible spectra revealed that the majority of spacers provided heterotrimers featuring extended π -electron delocalization. The new hybrid chromophores show a dramatically enhanced fluorescence compared with the DEE dimer and homo-trimer. This increase in emission intensity appears as a general feature of these systems: even if the spacer mol. is nonfluorescent, the corresponding hetero-trimer may show a strong emission. The redox properties of the new hybrid chromophores were determined by cyclic voltammetry (CV) and rotating disk voltammetry (RDV). In each case, the first 1-electron reduction step in the hetero-trimers appeared anodically shifted compared with DEE dimer and homo-trimer. With larger spacer chromophore extending into two dimensions, the anodic shift (by 240-490 mV) seems to originate from inductive effects of the two strongly electron-accepting DEE substituents rather than from extended π -electron conjugation along the oligomeric backbone, as had previously been observed for DEE substituted porphyrins.

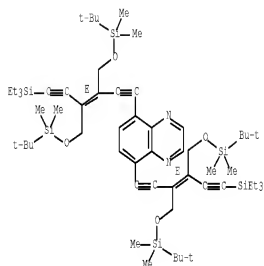
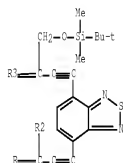
IT 477280-99-4P 477255-99-5P 477294-00-1P
477254-01-2P 477214-02-3P 477294-04-5P
477234-06-7P 477294-08-9P 477294-09-7P
477294-11-4P

RL: CFS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation, electrochem. properties and dramatically enhanced fluorescence
of compds. consisting of heterocoron. chromophores inserted as spacers into oligo(triacetylene)s)

RN 477293-90-4 CAPLUS

CN 2,1,3-Benzothiadiazole, 4,7-bis[(3E)-3,4-bis[[[(1,1-dimethylthyl)dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

PAGE 1-A

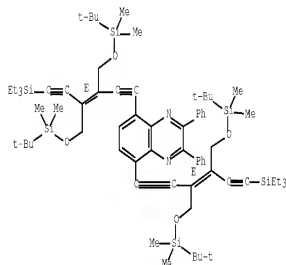


PAGE 2-A

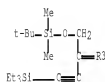


RN 477294-00-1 CAPLUS
CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]-2,3-diphenyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 3-A



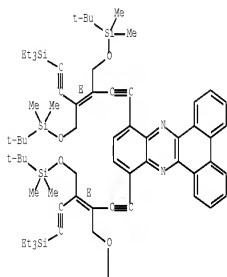
RN 477293-99-5 CAPLUS
CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (3CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 477294-01-2 CAPLUS
CN Dibenzo[a,c]phenazine, 10,13-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 2-A



RN 477294-04-5 CAPLUS
CN Zinc(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]di-pyrido[3,2-a:2',3'-c]phenazine-10,13-diyl]-, (T-4)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 477294-03-4
CMF C140 H212 N8 O8 Si12 Zn
CCI CCS

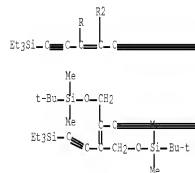
PAGE 2-A



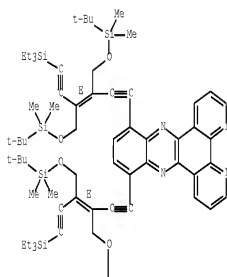
PAGE 1-A

RN 477294-02-3 CAPLUS
CN Dipyrdo[3,2-a:2',3'-c]phenazine, 10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

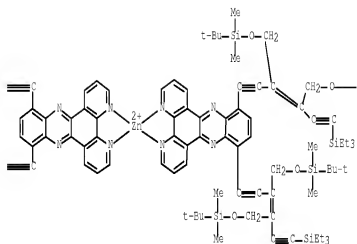
Double bond geometry as shown.



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PAGE 1-B



RN 477294-06-7 CAPLUS

CN Nickel(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-K[N4,N5]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

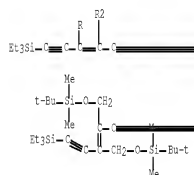
CM 1

CRN 477294-05-6

CMF C140 H212 N8 Ni 08 Si12

CCI	CCS
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PAGE 1-C



PAGE 2-A

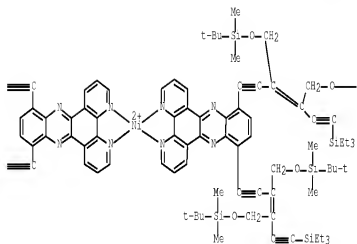


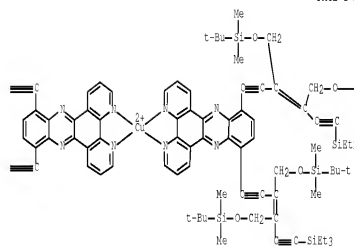
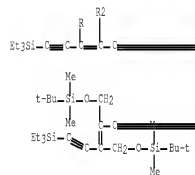
CM 2

CRN 37181-39-8

CMF C F3 03 S

PAGE 1-B





CM 2

CRN 14797-73-0

CME C1 04



RN 477294-08-9 CAPLUS
 CN Copper (2+), bis[[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-K]⁺], (T-4)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 477294-07-9

CME C140 H212 Cu N8 O8 Si12

CCI CCS



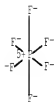


PAGE 2-A



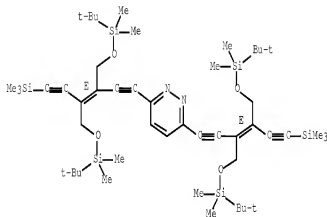
CN 2

CRN 16919-18-9
CMF P6 P
CCI CCS



RN 477294-09-0 CAPLUS
CN Pyridazine, 3,6-bis[(3E)-3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyne-1-yl]- (CA INDEX NAME)

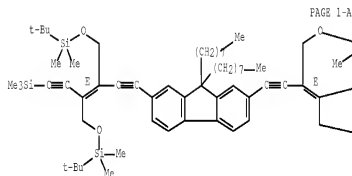
Double bond geometry as shown.



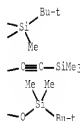
RN 477294-11-4 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(3,9-diocetyl-9H-fluorene-2,7-diyl)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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PAGE 1-B

OS.CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

18 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2002:539072 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 137:232177
TITLE: Anionic Cycloaromatization of 1-Aryl-3-hexen-1,5-diyne Initiated by Methoxide Addition: Synthesis of Phenanthridinones, Benzo[*c*]phenanthridinones, and Biaryls
AUTHOR(S): Wu, Ming-Jung; Lin, Chi-Pong; Lu, Wen-Der
CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan
SOURCE: Journal of Organic Chemistry (2002), 67(17), 5307-5312
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232177
AB Treatment of 2-((2)-6-substituted-3-hexene-1,5-diyne)benzonitriles with sodium methoxide in refluxing methanol in the presence of a polar aprotic solvent, such as DMSO, HMPA, THF, or 18-crown-6, gave phenanthridinones in 21-

77% yields. In these cases, addition of 10% DMSO into the reaction mixture gave the highest yield. On the other hand, methanolysis of 2-(2-(2-alkynylphenyl)ethyl)benzonitriles under the same reaction conditions gave benzo[c]phenanthridinones in 31-57% yields. Methanolysis of (2)-1-aryl-3-hexen-1,5-diyne in the presence of 2 equiv of tetrabutylammonium iodide gave biaryls in 14-64% yields. It is found that the reactions with aryl groups bearing electron-withdrawing groups proceeded at greater rates and gave better yields.

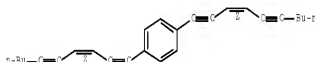
IT 457914-45-7P

RU: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(anionic cycloaromatization of 1-aryl-3-hexen-1,5-diyne initiated by addition of methanol)

RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di[(3Z)-3-decane-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2002:471478 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:310580

TITLE: Evaluation of ring-strain effects in cycloalkene-fused octadehydro[14]annulenes

AUTHOR(S): Boydston, A. J.; Laskoski, Matthew; Bunz, Uwe H. F.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Synlett (2002), (6), 981-983
CODEN: SYNLTT; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:310580

AB The possibility of ring strain as the cause of bond localization in metalloarene-fused octadehydro[14]annulenes is addressed. It was found that strain-induced bond localization is not observable in the mildly aromatic annulenes previously used to compare the degree of delocalization in CpCo(cyclobutadiene) relative to ferrocene and benzene.

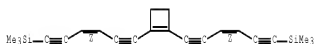
IT 472956-26-8P 472956-28-8P

RU: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(deprotection/cyclization; evaluation of ring-strain effects in cycloalkene-fused octadehydro[14]annulenes)

RN 472956-26-8 CAPLUS

CN Cyclobutene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

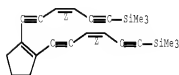
Double bond geometry as shown.



RN 472956-28-8 CAPLUS

CN Cyclopentene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2001:731976 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:53492

TITLE: Diatropicity of Dehydrobenzo[14]annulenes: Comparative Analysis of the Bond-Fixing Ability of Benzene on the Parent 3,4,7,8,9,10,13,14-Octadehydro[14]annulene

AUTHOR(S): Boydston, A. J.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Organic Letters (2001), 3(22), 3599-3601

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:53492

AB We report the synthesis of 3,4,7,8,9,10,13,14-octadehydro[14]annulene and detail a comparative aromaticity study with its benzannulated derivs. (e.g., benzo[e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene and dibenzo[a,e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene).

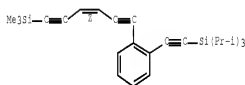
IT 381173-13-3P 381173-15-3P 381173-26-26

RU: PRE (Properties); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; diatropicity of dehydrobenzoannulenes)

RN 381173-13-3 CAPLUS

CN Benzene, 1-[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-(tris(1-methylsilyl)silyl)ethyl]- (CA INDEX NAME)

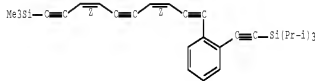
Double bond geometry as shown.



RN 381173-15-5 CAPLUS

CN Benzene, 1-[(3E,7E)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

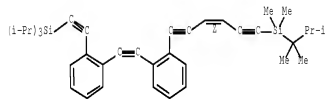
Double bond geometry as shown.



RN 381173-20-2 CAPLUS

CN Silane, [[2-[[2-[(3E)-6-(dimethyl(1,1,2-trimethylpropyl)silyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]phenyl]ethynyl]tris(1-methylethyl)- (3CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 25 OF 39 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:69640

TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units

AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490

PUBLISHER: EJOCHF; ISSN: 1434-193X

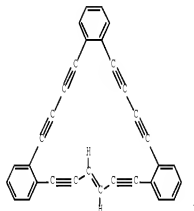
WILEY-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:69640

GI



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., 1, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. IN NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 systems) and antiarom. (4n systems) behavior, in spite of their large size and extensive benzannulation.

IT 214628-16-7H 214628-17-8P 214628-18-9P 214628-19-4P

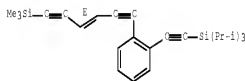
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)

RN 214628-16-7 CAPLUS

CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

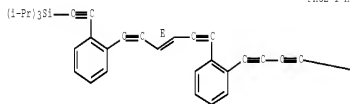
Double bond geometry as shown.



RN 214628-17-8 CAPLUS

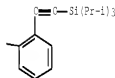
CN Silane, tris(1-methylethyl)[[2-[(3E)-6-(2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (3CI) (CA INDEX NAME)

Double bond geometry as shown.



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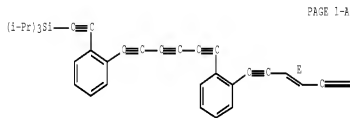
PAGE 1-B



RN 214620-18-9 CAPLUS

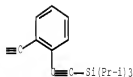
CN Silane, tris(1-methylethyl)[[2-{6-[[3E]-6-(2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatrienyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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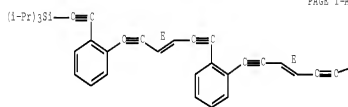
PAGE 1-B



RN 383404-38-4 CAPLUS

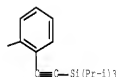
CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis(tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



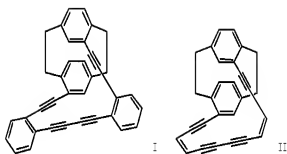
PAGE 1-A

PAGE 1-B



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

18 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 2001:664308 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 136:5789
TITLE: [2.2]Paracyclophane/dehydrobenzoannulene hybrids: Transannular delocalization in open-circuited conjugated macrocycles
AUTHOR(S): Boydston, A. J.; Bondarenko, Lidija; Dix, Ina; Weakley, Timothy J. R.; Hopf, Henning; Haley, Michael M.
CORPORATE SOURCE: Institut für Organische Chemie, Technische Universität Braunschweig, Braunschweig, 38106, Germany
SOURCE: Angewandte Chemie, International Edition (2001), 40 (16), 2986-2989
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:5789
GI



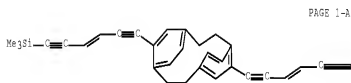
AB Formylation and following alkylation of dibromoparacyclophane gave dialkynylparacyclophane as key for the synthesis of (2,2)paracyclophane/dehydrobenzoannulene hybrids I and II. I and II were assembled by Pd-catalyzed cross-coupling of iodoarene and chloroalkene with dialkynylparacyclophane and subsequent cyclization. The study of the transannular delocalization in open-circuited conjugated macrocycles using optical properties and the elucidation of solid-stated structure of II by x-ray crystallog. (monoclinic, P2₁/n, a 9.505(2), b 15.077(2), c 13.687(2)Å, β 96.608(8), V 1939.3(6) Å³, Z 4) are reported.

IT 375366-59-9:

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PRCP (Preparation); RACT (Reactant or reagent)
(preparation and transannular delocalization of open-circuited conjugated paracyclophane/dehydrobenzoannulene macrocycles)

RN 375366-59-9 CAPLUS

CN Tricyclo[9.2.2.2.2.4,7]hexadeca-4,6,10,12,13,15-hexaene, 5,11-bis[5-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-, stereoisomer (CA INDEX NAME)



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PAGE 1-B

OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2001:481503 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 135:211133
TITLE: Organometallic Dehydro[14]annulenes Containing Vollhardt's Cyclobutadiene: Are CpCo-Complexed Cyclobutadienes More Aromatic than Benzene?
AUTHOR(S): Lastoski, Matthew; Smith, Mark D.; Morton, Jason G. M.; Bunz, Uwe H. F.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC, 29208, USA
SOURCE: Journal of Organic Chemistry (2001), 66(15), 5174-5181
CODEN: JOCEAH; ISSN: 0022-5263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:211133

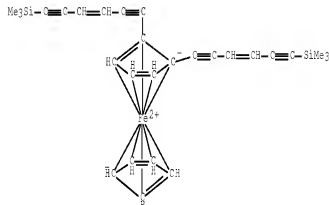
AB Pd-catalyzed coupling of [1,2-diethynyl-3,4-bis(trimethylsilyl)cyclobutadiene][cyclopentadienyl]cobalt to a series of 1-iodo-2-(trimethylsilyl)ethynylbenzenes and 1-chloro-4-trimethylsilylbut-1-ene-3-yne is followed by desilylation with potassium carbonate. Cu(OAc)₂-promoted oxidative ring closure leads to dehydro[14]annulenes and dehydro[14]benzoannulenes fused to a cyclobutadiene(cyclopentadienylcobalt) complex. Five of these fused dehydroannulenes were structurally characterized. 1H NMR spectroscopy of the organometallic dehydro[14]annulenes incorporating the (bis(trimethylsilyl)cyclobutadiene)(cyclopentadienylcobalt) unit suggested that the aromaticity of the fused cyclobutadienes complex might be stronger than that of benzene according to the ring-current criterion.

IT 350586-85-5 350586-94-6

RL: PRP (Properties)
(NMR and aromaticity of)

RN 350586-85-5 CAPLUS

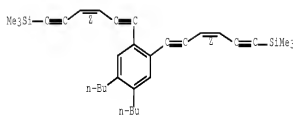
CN Ferrocene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)



RN 350586-94-6 CAPLUS

CN Silane, [(4,5-dibutyl-1,2-phenylene)di-(3Z)-3-hexene-1,5-diyn-6,1-diyl]bis(trimethyl- (9CI) (CA INDEX NAME)

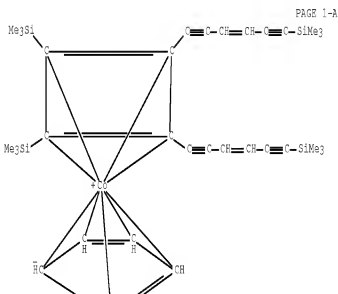
Double bond geometry as shown.



IT 358365-18-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation, desilylation, and sequential copper-catalyzed oxidative ring
 closure of)

RN 358365-18-1 CAPLUS

CN Cobalt, [[[1,2,3,4-η]-3,4-bis(trimethylsilyl)-1,3-cyclobutadiene-1,2-
 diyl]di-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis(trimethylsilane)](η⁵-2,4-
 cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



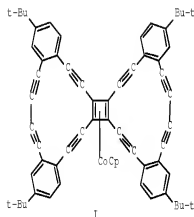
PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 27 THERE ARE 27 CAPLUS RECORDS THAT CITE THIS
 RECORD (28 CITINGS)
 REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

18 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2009 ACS on SIN
 ACCESSION NUMBER: 2001:318816 CAPLUS Full-text
 DOCUMENT NUMBER: 135:92741
 TITLE: Concave butterfly-shaped organometallic hydrocarbons?
 AUTHOR(S): Laskoski, Matthew; Roidl, Gaby; Smith, Mark D.; Bunz, Uwe H. F.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, The
 University of South Carolina, Columbia, SC, 29208, USA
 SOURCE: Argawandte Chania, International Edition (2001),
 40(8), 1460-1463
 CODEN: ACFE33; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:92741
 GI

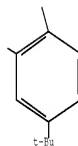
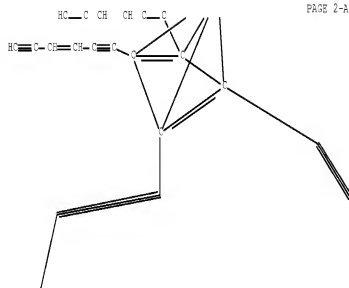
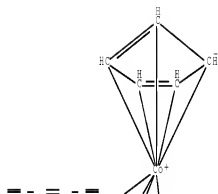


AB The preparation of title novel large concave organometallic hydrocarbon with a
 central tetraethynylcyclobutadiene(cyclopentadienylcobalt) core, e.g. I,
 starting from tetraalkynylcyclobutadiene cobalt complex in five steps is
 described. The crystal structure of I was determined

IT 349453-21-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and cyclization of)

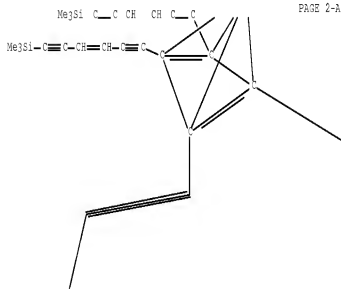
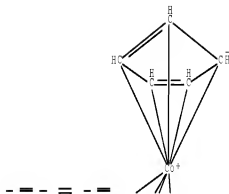
RN 349453-21-0 CAPLUS

CN Cobalt, (η⁵-2,4-cyclopentadien-1-yl)((1,2,2a,18a-η)-
 3,4,9,10,11,12,17,18-octadecahydro-7,14-bis(1,1-dimethylethyl)-1,2-di-(3Z)-3-
 hexene-1,5-diyndibenzocyclobuta[a]cyclooctatetradecene)- (9CI) (CA
 INDEX NAME)



IT 349453-00-9P
 RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACI
 (Reactant or reagent)
 (preparation and desilylation of)
 RN 349453-00-9 CAPLUS
 CN Cobalt, (η⁵-2,4-cyclopentadien-1-yl)[{[(1,2,2a,18a-η)-
 3,4,9,10,11,12,17,18-octadehydro-7,14-bis(1,1-
 dimethylethyl)dibenzo[a,1]cyclobuta[e]cyclotetradecene-1,2-diyl]di-(3Z)-3-

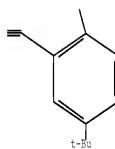
PAGE 1-A



PAGE 2-A



PAGE 3-A

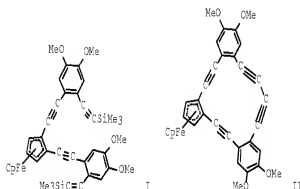
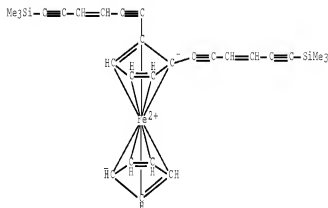


PAGE 3-B

OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)
 REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

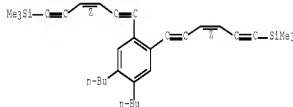
18 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2001:293307 CAPLUS Full-text
 DOCUMENT NUMBER: 135:107433

TITLE: Is ferrocene more aromatic than benzene?
 AUTHOR(S): Laskoski, Matthew; Steffen, Winfried; Smith, Mark D.;
 Bunz, Uwe H. F.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, The
 University of South Carolina, Columbia, SC, 29208, USA
 SOURCE: Chemical Communications (Cambridge, United Kingdom)
 (2001), (8), 691-692
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:107433
 GI



RN 350586-94-6 CAPLUS
 CN Silane, [(4,5-dibutyl-1,2-phenylene)di-(3,2)-3-hexene-1,5-diyne-6,1-diyl]bis(trimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



AB A combination of Pd-catalyzed arene-alkynyl couplings and Cu(OAc)2-promoted
 internal alkyne dimerization furnishes novel ferrocene-based dehydroannulenes
 in high yield. Thus, palladium-copper catalyzed coupling of 1,2-
 diethynylferrocene 1-1-2,3-(MeO)2C6H2C.tpbond.CSiMe3 gave 3% tetrayne I
 which on K2CO3/MeOH mediated desilylation followed by cyclization with
 Cu(OAc)2/MeCN gave 4% dehydroannulene II.
 IT 350586-85-5P 350586-94-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation, desilylation, and sequential copper catalyzed cyclization of)
 RN 350586-85-5 CAPLUS
 CN Ferrocene, 1,2-bis[(3,2)-6-(trimethylsilyl)-3-hexene-1,5-diyne]- (9CI)
 (CA INDEX NAME)

CS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS
 RECORD (28 CITINGS)
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

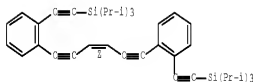
18 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:832492 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 134:310920
 TITLE: Bis(enediynes) Macrocycles: Synthesis, Reactivity, and
 Structural Analysis
 AUTHOR(S): Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley,
 T. J. R.; Haley, M. M.
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene,
 OR, 97403-1253, USA
 SOURCE: Tetrahedron (2000), 56(49), 9561-9588
 CODEN: TETRAE; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:310920
 AB The authors describe the syntheses of five macrocycles possessing two enediynes
 warheads, along with the structural and thermal analyses of these
 bis(enediynes) compds. The solid-state packing of one of the compds. suggests
 the possibility for the mol. to undergo a topochem. diacetylene polymerization
 IT 335379-80-6P 335379-80-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of bis(enediynes) macrocycles)

RN 335378-20-6 CAPLUS

CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)]

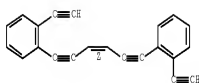
Double bond geometry as shown.



RN 335378-30-8 CAPLUS

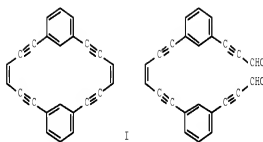
CN Benzene, 1,1'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2-ethynyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:767122 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 134:71381
TITLE: Synthesis and structure of a new [6.6]metacyclophane with enediynes bridges
AUTHOR(S): Srinivasan, Manivannan; Sankararaman, Sethuraman; Dix, Ina; Jones, Peter G.
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, 600 036, India
SOURCE: Organic Letters (2000), 2(24), 3849-3851
CODEN: ORLEP7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:71381
GI



AB Synthesis and structure of a novel [6.6]metacyclophane with enediynes bridges I is reported. I was prepared by reacting 1,3-diethynylbenzene with EtMgBr/THF and DMT to give the monoaldehyde. The monoaldehyde was subsequently converted to the acetal, coupled with ClCH2CHCl2 to give bis-acetal, which was hydrolyzed to the dialdehyde II. II underwent McMurry coupling using TiCl3 and Zn-Cu couple in DME to give I in 69% yield.

IT 335716-90-AP 315716-91-7P

RL: RCT (Reactant); SEN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and crystal structure of metacyclophane with enediynes bridges)

RN 315716-90-6 CAPLUS

CN 1,3-Dioxolane, 2,2'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene-2,1-ethynediyl)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



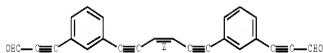
PAGE 1-B



RN 315716-91-7 CAPLUS

CN 2-Propynyl, 3,3'-[(3Z)-3-hexene-1,5-diyne-1,6-diyl]-3,1-phenylene]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1999:625317 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:337377

TITLE: Modulation of π -electron conjugation in oligo(triarylene) chromophores by incorporation of a central spacer

AUTHOR(S): Martin, Rainer E.; Wytko, Jennifer A.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium für Organische Chemie, ETH-Zentrum, Zurich, CH-8032, Germany

SOURCE: Helvetica Chimica Acta (1999), 82(9), 1470-1485

CODEN: HCAQAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of trimeric hybrid oligomers was prepared by insertion of different hetero-spacers between two (E)-hex-3-ene-1,5-diyne (E = 1,2-diethynylethene, DEE) moieties, and the optical and electrochem. properties of the resulting π -conjugated materials were compared to those of the DEE dimer and trimer, which formally contain a DEE moiety as homo-spacer. The hetero-spacers were: benzenoid (phenylene, naphthalene, biphenylene, anthracene), π -electron-deficient (pyrazine, pyridine) and π -electron-rich (thiophene, furan) aromatic rings, and trans-Pt(PPh₃)₂. The hybrid oligomers were synthesized using the method of K. Sonogashira et al. (1978), i.e., cross-coupling between mono-deprotected DEE and the appropriately bis-functionalized spacer. UV/VIS data revealed that the majority of the hetero-spacers were less effective than the homo-spacer DEE in facilitating π -electron delocalization along the linearly conjugated oligomeric backbone. With increasing degree of benzenoid aromaticity in the hetero-spacer, the electronic communication between the terminal DEE moieties in the hybrid oligomers was reduced. As a remarkable exception, a large bathochromic shift of the longest-wavelength absorption maximum, which is indicative of enhanced π -electron delocalization, was obtained upon introducing an anthracene-9,10-diyl moiety as hetero-spacer. Electrochem. studies by cyclic and steady-state voltammetry confirmed the limited extent of π -electron delocalization in the majority of the hybrid oligomers. The fluorescence properties of many of the DEE hybrid materials were dramatically enhanced upon incorporation of the heterospacers. The heterocyclic derivs. containing pyridine, pyrazine, or thiophene spacers, resp., displayed a strong fluorescence emission, demonstrating the value of combining repeat units to modulate oligomeric and polymeric properties. The pyridine derivative provided an interesting example of a mol. system, in which both the electronic absorption and emission characteristics can be reversibly switched as a function of pH.

II 249616-79-39, 4-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diyne]benzene 249616-82-89,

2,6-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diyne]naphthalene 249616-33-39, 9,10-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diyne]anthracene 249616-84-89 249616-87-39, 1,4-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diyne]2,3,5,6-tetramethylbenzene 249616-88-49 249616-49-59, 2,5-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diyne]pyrazine 249616-90-89 249616-91-90, 2,5-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diyne]furan

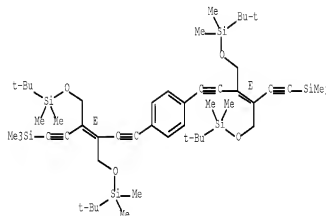
RI: PREP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and modulation of π -electron conjugation in oligoarylene chromophores by central spacer with variable electron d.)

RN 249616-79-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E,6'E)-(SCI) (CA INDEX NAME)

Double bond geometry as shown.

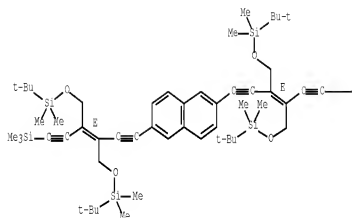


RN 249616-82-88 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,6-naphthalenediyl-di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E,6'E)-(SCI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

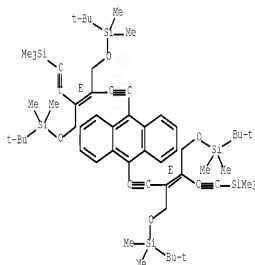


PAGE 1-B

—SiMe₃

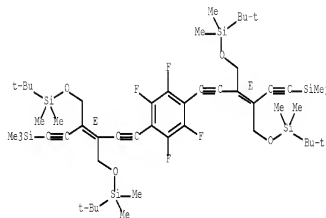
RN 249616-83-9 CAPLUS
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-((9,10-anthracenediyl)di-2,1-ethynediyl)bis(2,2,3,3,10,10,11,11-octamethyl-7-((trimethylsilyl)ethynyl)-, (6E,6'E)- (3CI) (CA INDEX NAME)

Double bond geometry as shown.



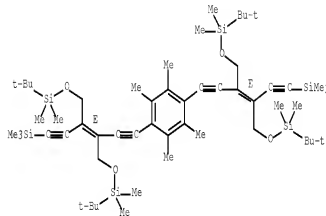
RN 249616-84-0 CAPLUS
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-((2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl)bis(2,2,3,3,10,10,11,11-octamethyl-7-((trimethylsilyl)ethynyl)-, (6E,6'E)- (3CI) (CA INDEX NAME)

Double bond geometry as shown.



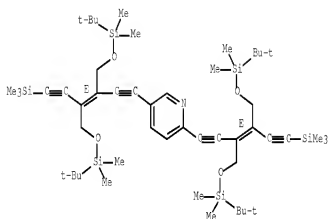
RN 249616-87-3 CAPLUS
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-((2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl)bis(2,2,3,3,10,10,11,11-octamethyl-7-((trimethylsilyl)ethynyl)-, (6E,6'E)- (3CI) (CA INDEX NAME)

Double bond geometry as shown.



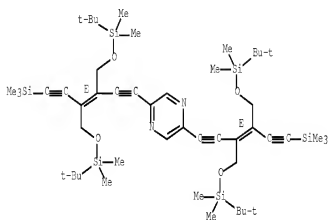
RN 249616-88-4 CAPLUS
CN Pyridine, 2,5-bis[[3E]-3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxymethyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



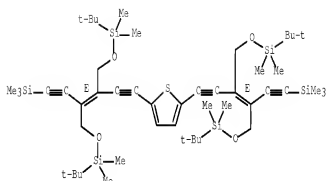
RN 249616-89-5 CAPLUS
CN Pyrazine, 2,5-bis[(3E)-3,4-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyne-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



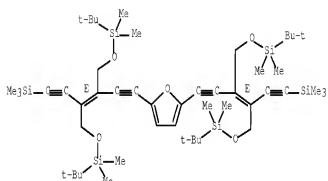
RN 249616-90-8 CAPLUS
CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,5-thiophenediyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (SCI) (CA INDEX NAME)

Double bond geometry as shown.



RN 249616-91-9 CAPLUS
CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,5-furandiyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (SCI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS RECORD (29 CITINGS)
REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 1996:756297 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 130:118607
TITLE: Porphyrin-[(E)-1,2-diethynylethane] scaffolding. Synthesis and optical and electrochemical properties of multianometer-sized porphyrin arrays
AUTHOR(S): Wytko, Jennifer; Berl, Volker; McLaughlin, Mark; Tykwinski, Rik R.; Schreiber, Martin; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice
CORPORATE SOURCE: Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.
SOURCE: Helvetica Chimica Acta (1998), 81(11), 1964-1977
CODEN: HUCANV; ISSN: 0010-019X
PUBLISHER: Verlag Helvetica Chimica Acta AG
DOCUMENT TYPE: Journal

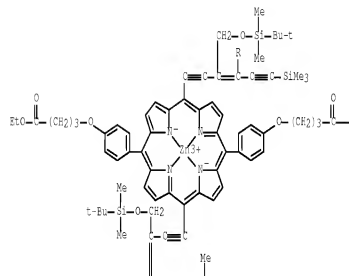
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two series of linearly conjugated hybrid materials, consisting of (E)-1,2-diethynylethene (DEE; hex-3-ene-1,5-diyne) and Zn(II) porphyrin components, were prepared by Pd0-catalyzed cross-coupling reactions. In I series, 1 or 2 DEE substituents were introduced into the meso-positions of the Zn(II) porphyrins, leading from Zn 5,15-bis[[(ethoxycarbonyl)propoxy]phenyl]porphinate (I) to I and II (n = 1; R = SiMe2tBu). The second series contains the linearly π -conjugated mol. rods III (n = 1-3) that span a length range from 23 Å for III (n = 1) to 53 Å for III (n = 3). The larger rods III (n = 2 and 3) consist of 2 or 3 porphyrin moieties, resp., that are bridged at the meso-positions by trans-enediynediyl (hex-3-ene-1,5-diyne-1,6-diyl) linkers. The UV/Vis spectra in the series I, II, and III (n = 1) showed a strong bathochromic shift of both Soret and Q bands of the Zn(II) porphyrin as a result of the addition of DEE substituents. Upon changing from I to II, the Q band was further bathochromically shifted, whereas the Soret band remained nearly at the same position but became broadened and displayed a shoulder on the lower-wavelength edge as a result of excitonic coupling. The close resemblance between the UV/Vis spectra of III (n = 2 and 3) suggests that saturation of the optical properties in the oligomeric series already occurs at the stage of dimeric III (n = 2). Stationary voltammetric investigations showed that the DEE substituents act as strong electron acceptors which induce large anodic shifts in the 1st reduction potential upon changing from I to II ($\Delta E = 190$ mV) and to III (n = 1) ($\Delta E = 340$ mV). Increasing the number of porphyrin moieties upon changing from III (n = 1) to III (n = 2) had no effect on the 1st reduction potential yet the 1st oxidation potential was substantially lowered ($\Delta E = 110$ mV). Large differences in the potentials for 1-electron oxidation of the 2 porphyrin moieties in III (n = 2) ($\Delta E = 200$ mV) confirmed the existence of substantial electronic communication between the 2 macrocycles across the trans-enediynediyl bridge.

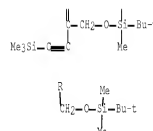
IT 219483-26-3 219483-27-3
 RL: FNU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
 (elec. potential of couple containing)

RN 219483-26-8 CAPLUS

CN Zinc(1+), [diethyl 4,4'-[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl-
 wK21,wK22,wK23,wK24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)



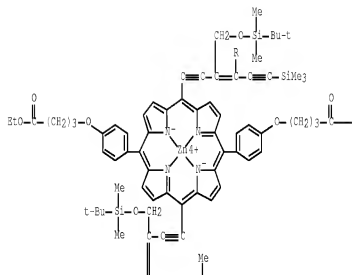
—OEt



RN 219483-27-9 CAPLUS

CN Zinc(2+), [[diethyl 4,4'-[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl-
 wK21,wK22,wK23,wK24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)

PAGE 1-A

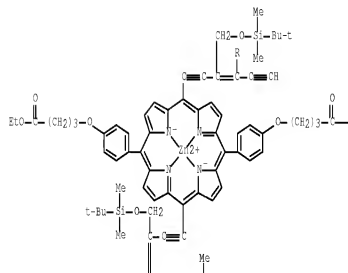


PAGE 1-B

—OEt

porphine-5,15-diyl-K021,K022,K023,K024[bis(4,1-phenylenaoxy)]bis[butanoato]](2-)-, (SP-4-1)- (9CI) (CA INDEX NAME)

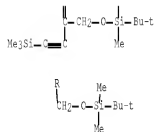
PAGE 1-A



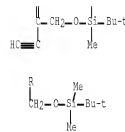
PAGE 1-B

—OEt

PAGE 2-A



PAGE 2-A

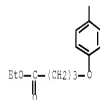


IT 213483-13-9P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of reactant for preparation zinc porphyrin diethylethene monomeric, dimeric, and trimeric complexes and NMR)
 RN 219483-18-8 CAPJUS
 CN Zinc, [[diethyl 4,4'-[[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]-21H,23H-

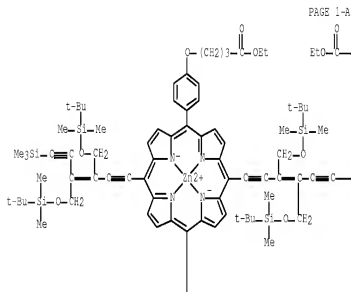
IT 213483-13-9P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, UV spectra, electrochem. redox behavior and conversion to

RM 219483-19-9 CAPLUS
trinnuclear complex and NMR)

CN Zinc, [μ-[[[tetraethyl 4,4',4'',4'''-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexeno-1,5-diyne-1,6-diyl]bis[[[20-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexeno-1,5-diyne]]-21H,23H-porphine-10,5,15-triyl-κN21,κN22,κN23,κN24]-4,1-phenyleneoxy]]tetrakis[butanoato]](4-)]di- (3CI) (CA INDEX NAME)



PAGE 2-A



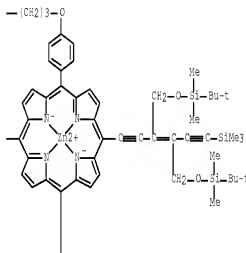
PAGE 1-A



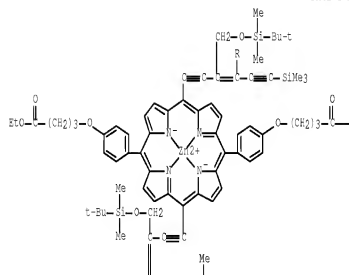
PAGE 2-B

IT 219483-15-5G
R1: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, UV spectra, electrochem. redox behavior, and deprotection and NMR)

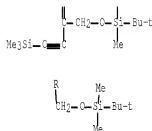
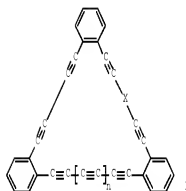
RM 219483-15-5 CAPLUS
CN Zinc, [[diethyl 4,4'-[[[10,20-bis[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexeno-1,4-diynyl]-21H,23H-porphine-5,15-diyl-κN21,κN22,κN23,κN24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (3CI) (CA INDEX NAME)



PAGE 1-B



PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)

REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 1998:606810 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:302407

ORIGINAL REFERENCE NO.: 129:61683a,61686a

TITLE: Synthesis of expanded planar dehydrobenzoannulenes: weakly diatropic, weakly paratropic, or atropic?

AUTHOR(S): Wan, M. Brad; Kimball, David B.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA

SOURCE: Tetrahedron Letters (1998), 39(38), 6795-6798

CODEN: TETLEA; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:302407

GI

AB Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes I [X = C, tpbond, C, (E)-CH=CH; n = 0,1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannulation, dehydrobenzoannulenes possess weak induced ring currents.

IT 214628-16-7; 214628-17-8; 214628-18-9

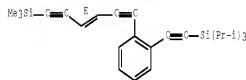
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of expanded planar dehydrobenzoannulenes with triacetylenic linkages)

RN 214628-16-7 CAPLUS

CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

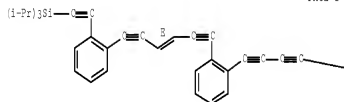
Double bond geometry as shown.



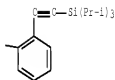
RN 214628-17-8 CAPLUS

CN Silane, tris(1-methylethyl)[(2-[(3E)-6-(2-(4-(2-[tris(1-methylethyl)silyl]ethynyl)phenyl)-1,3-butadiynyl]phenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]- (3CI) (CA INDEX NAME)

Double bond geometry as shown.



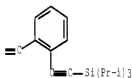
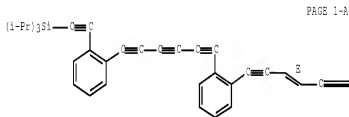
PAGE 1-A



RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[(2-(6-{2-[(3E)-6-{2-[(tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:680471 CAPLUS Full-text

DOCUMENT NUMBER: 121:280471

ORIGINAL REFERENCE NO.: 121:51203a,51206a

TITLE: Preparation of dynemicin analogs as bactericides and antitumor agents

INVENTOR(S): Smith, Adrian L.; Hwang, Chan Kou; Wenderborn, Sebastian V.; Nicolaou, Kyriacos C.; Schreiner, Erwin P.; Stahl, Wilhelm; Dai, Wei Ming; Mailgrea, Peter E.; Suzuki, Toshio

PATENT ASSIGNER(S): Scripps Research Institute, USA

SOURCE: U.S., 114 pp. Cont.-in-part of U.S.Ser. No. 886,984,abandoned.

COKEY: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

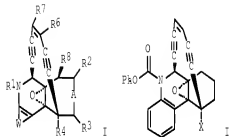
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5261710	A	19940125	US 1992-939104	19920901
US 5276259	A	19940104	US 1992-886984	19920521
US 5500432	A	19960319	US 1993-46626	19930414
WO 9323046	A1	19931125	WO 1993-US4708	19930518
W: AU, CA, FI, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343607	A	19931213	AU 1993-43807	19930518
AU 680418	B2	19970731		
EP 641207	A1	19950308	EP 1993-91366	19930518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07506037	T	19950907	JP 1994-503616	19930518
US 5527605	A	19960618	US 1994-184580	19940121
FI 9405427	A	19950118	FI 1994-5427	19941118
NO 9404429	A	19950123	NO 1994-4429	19941118
PRIORITY APPLN. INFO.:				
			US 1990-562269	B2 19900801
			US 1991-673199	B2 19910321
			US 1991-734613	B2 19910723
			US 1991-768225	B2 19911105
			US 1992-886984	B2 19920521
			US 1992-939104	A2 19920901
			WO 1993-US4708	A 19930518

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:280471

GI



AB The title compts. I [A = double or single bond; R1 = H, alkyl, phenoxycarbonyl, etc.; R2 = H, carbonyl, hydroxylmethyl, etc.; R3 = H, alkoxy; R4 = H, hydroxyl, alkoxy, etc.; R6 and R7 are each H or together with the intervening vinylene group form a one, two or three fused aromatic six-membered ring system; W together with the bonded, intervening, vinylene group (i.e., the unsatd. carbon atoms bonded to W) forms a substituted aromatic hydrocarbyl ring system containing 1, 2, or 3 six-membered rings such that said fused ring compound contains 3, 4, or 5 fused 6-membered rings all but two of which rings are aromatic, and in which that aromatic hydrocarbyl ring

system, W, is joined [a,b] to the structure shown; R8 = H, or Me; a proviso is given) are prepared Title compound II (X = OH) (preparation given) in vitro exhibited IC50 of 6.3 x 10-6 M against a variety of cancer cell lines. II (X = H) in vitro exhibited IC50 of 5.0 x 10-6 M against a variety of cancer cell lines.

IT 144227-80-UP 144227-81-UP
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

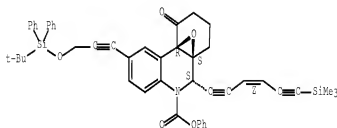
(preparation and reaction of, in preparation of bactericide and antitumor agent)

RN 144227-80-0 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid, 2-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-propynyl]-7,8,9,10-tetrahydro-10-oxo-6-[6-(trimethylsilyl)-3-hexene-1,5-diynyl]-, phenyl ester, (6a(Z),6aβ,10aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

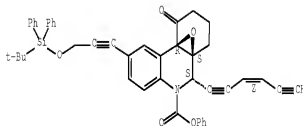


RN 144227-81-1 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid, 2-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-propynyl]-6-(3-hexene-1,5-diynyl)-7,8,9,10-tetrahydro-10-oxo-, phenyl ester, [6a(Z),6aβ,10aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:680470 CAPLUS R11-text

DOCUMENT NUMBER: 121:280470

ORIGINAL REFERENCE NO.: 121:51202h,51203a

TITLE: Preparation of dynemicin analogs as DNA binding, antibiotic, and antitumor agents.

INVENTOR(S): Smith, Adrian L.; Hwang, Chan Kou; Wendeborn, Sebastian V.; Nicolau, Kyriacos C.; Schreiner, Erwin P.; Stahl, Wilhelm; Dai, Wei Ming; Mallgren, Peter D.; Suzuki, Toshie

PATENT ASSIGNEE(S): Scripps Research Institute, USA

SOURCE: U.S., 109 pp. Cont.-in-part of U.S. Ser. No. 788,225.

CODEN: USKXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5276159	A	19940104	US 1992-886984	19920521
US 5281710	A	19940125	US 1992-939104	19920901
US 5500432	A	19960319	US 1993-46626	19930414
WO 9323046	A1	19931125	WO 1993-054708	19930518
W: AU, CA, FI, JP, WO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343607	A	19931213	AU 1993-43807	19930518
AU 680418	B2	19970731		
EP 641207	A1	19950308	EP 1993-91366	19930518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 07508037	T	19950907	JP 1994-503816	19930518
US 5527805	A	19960618	US 1994-184580	19940121
FI 9405427	A	19950118	FI 1994-5427	19941118
NO 9404429	A	19950123	NO 1994-4429	19941118
PRIORITY APPLN. INFO.:				
			US 1990-562269	B2 19900801
			US 1991-673199	B2 19910321
			US 1991-734613	B2 19910723
			US 1991-788225	A2 19911105
			US 1992-886984	B2 19920521
			US 1992-939104	B2 19920901
			WO 1993-054708	A 19930518

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN L8US DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:280470

G1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R1 = H, alkyl, PhO2C, PhCH2O2C, 9-fluorenylmethoxycarbonyl, o-nitrobenzylloxycarbonyl, (substituted) alkoxy-carbonyl; R2 = H, CO2H, CH2OH, carbonyloxyalkyl; R3 = H, alkoxy; R4 = H, OH, alkoxy, oxoacetic acid, oxoacetic hydrocarbyl or benzyl ester, oxoacetic amide, acyloxy, etc.; R6, R7 = H; R6R7 = atoms to form a 1, 2, or 3-fused aromatic 6-membered ring system; R8 = H, Me, with provisos; A = double or single bond; W = atoms to form an aromatic hydrocarbyl ring system containing 1, 2, or 3 six-membered rings such that the fused ring compound contains 3, 4, or 5 fused rings, all but 2 of which are aromatic], were prepared Chimeric compds. having the fused ring system compound as an aglycon bonded to (i) a sugar moiety as the oligosaccharide portion or (ii) a monoclonal antibody or antibody combining site portion thereof that immunoreacts with target tumor cells are also

disclosed. Thus, title compound III (preparable via claimed compound II) inhibited Molt-4 T-cell leukemia with IC50 = 2.0 + 10-14 M; III was 1-8 orders of magnitude more active against tumor cells than against normal cells. I structure-activity relationships are discussed.

IT 144127-81-1P

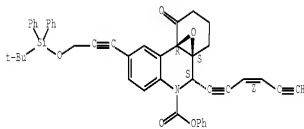
RI: SPW (Synthetic preparation); PREP (Preparation)
(preparation of, as DNA binding, antibiotic, and antitumor agent)

RN 144127-81-1 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid,
2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propenyl]-6-(3-hexene-1,5-dienyl)-7,8,9,10-tetrahydro-10-oxo-, phenyl ester,
[6a(2),6aβ,10aβ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



IT 144127-80-0P

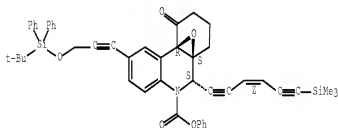
RI: SPW (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for DNA binding, antibiotic, and antitumor dynemicin analog)

RN 144127-80-0 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid,
2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propenyl]-7,8,9,10-tetrahydro-10-oxo-6-[6-(trimethylsilyl)-3-hexene-1,5-dienyl]-, phenyl ester, [6a(2),6aβ,10aβ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)

L8 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:633659 CAPLUS Full-text

DOCUMENT NUMBER: 117:233659

ORIGINAL REFERENCE NO.: 117:40395a,40398a

TITLE: Molecular design and chemical synthesis of potent enedynes. 1. Dynemicin model systems equipped with N-tethered triggering devices

AUTHOR(S): Niccolau, K. C.; Malligres, P.; Suzuki, T.; Wendeborn, S. V.; Dai, W. M.; Chacha, R. K.

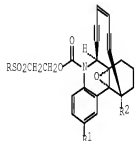
CORPORATE SOURCE: Dep. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA

SOURCE: Journal of the American Chemical Society (1992), 114(23), 8990-907
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB In this article the mol. design and chemical synthesis of a series of enedynes I (R = Ph, 1-naphthyl, 2-naphthyl; R1 = H, MeO, HOCH2CH2O, HOCH2C(CH2OH)2; R2 = H, MeO, HOCH2CH2O) related to the dynemicin A structure and carrying N-tethered triggering devices are described. The design envisioned the ((arylsulfonyl)ethoxy)carbonyl group attached at the nitrogen atom as a triggering device for the Bergman cycloaromatization reaction because of its ability to undergo β-elimination under basic conditions, liberating the labile free amine intermediate. A number of tethering groups on the aromatic ring were also installed in these systems for future incorporation of other desirable moieties such as delivery systems and solubility enhancers. Bergman cycloaromatization expts. under basic and acidic conditions demonstrated the abilities of these compds. to generate benzenoid diradicals. A number of potent DNA-cleaving compds. and cytotoxic agents emerged from these studies.

IT 144127-80-0P

RI: RCT (Reactant); SPW (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

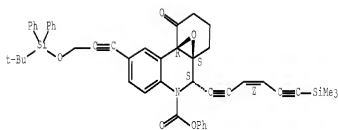
(preparation and desilylation of)

RN 144127-80-0 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid,
2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propenyl]-7,8,9,10-tetrahydro-10-oxo-6-[6-(trimethylsilyl)-3-hexene-1,5-dienyl]-, phenyl ester, [6a(2),6aβ,10aβ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



IT 144127-61-10

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

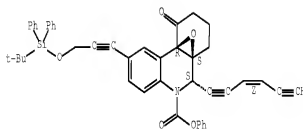
(preparation and intramol. cycloaddn. reaction of, epoxyhexamethylenephosphanthridine from)

RN 144127-61-1 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid, 2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propynyl]-6-(3-hexene-1,5-diynyl)-7,8,9,10-tetrahydro-10-oxo-, phenyl ester, [6a(2),6aβ,10aβ]- (9C1) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (31 CITINGS)

L8 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1989:212183 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 110:212183

ORIGINAL REFERENCE NO.: 110:35199a,35202a

TITLE: A short route to dehydro[12]annulenes

AUTHOR(S): Huynh Chanh; Linstrumelle, Gerard

CORPORATE SOURCE: Lab. Chim., Ec. Norm. Super., Paris, 75231, Fr.

SOURCE: Tetrahedron (1988), 44(20), 6337-44

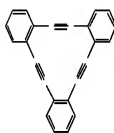
CODEN: TETRA8; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:212183

GI



I

AB A novel synthesis of dehydro[12]annulenes from o-BrC6H4 is based on selective Pd(0)-Cu(I) coupling reactions of aryl and vinyl halides with terminal acetylenes. Thus, coupling reaction of o-BrC6H4 with HC.tplbond.CMe2OH gave 63% o-BrC6H4C.tplbond.CMe2OH. Cleavage with NaOH followed by in situ trimerization gave 36% dehydroannulene 1.

IT 120651-32-39

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and desilylation of)

RN 120651-32-3 CAPLUS

CN Silane, [6-(2-(4-chloro-3-buten-1-ynyl)phenyl)-3-hexene-1,5-diynyl]trimethyl-, (Z,Z)- (9C1) (CA INDEX NAME)

Double bond geometry as shown.



IT 120651-34-79

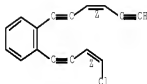
RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and intramol. coupling reaction of, dehydroannulene from)

RN 120651-36-7 CAPLUS

CN Benzene, 1-(4-chloro-3-buten-1-ynyl)-2-(3-hexene-1,5-diynyl)-, (Z,Z)- (9C1) (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

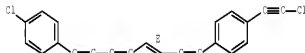
ACCESSION NUMBER: 1988:79350 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 68:76330
 ORIGINAL REFERENCE NO.: 68:15123a,15126a
 TITLE: Interaction of diiodoethylene with copper acetylides
 AUTHOR(S): Ukhir, L. Yu.; Sladkov, A. M.; Gorskoy, V. I.
 CORPORATE SOURCE: Inst. Elementorg. Soedin, Moscow, USSR
 SOURCE: Zhurnal Organicheskoi Khimii (1968), 4(1), 25-7
 CODEN: ZORXAE; ISSN: 0514-7492
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian

AB Reaction of trans-diiodoethylene (I) with Cu acetylides gave the condensation products of general formula $RC.tpbond.CHC:CHI$ (IIa) or $RC.tpbond.CHC:CHC.tpbond.CR$ (IIb). The structure of products was confirmed by ir and mass spectroscopy; trans configuration of the double bond was preserved. For example, a mixture of 3.29 g. (PAC.tpbond.C)2Cu, 2.78 g. I, and 100 ml. $HCONH_2$ was stirred 4 hrs. at 90° and then refluxed 2 hrs. Cooling, filtration, and addition of H_2O to the filtrate precipitated 56% IIb (R = Ph) m. 111-12° (heptane). Similarly, IIb (R = Bu) b4 117°, n24D 1.5173 was prepared. Boiling 23.4 g. (BuC.tpbond.C)2Cu with 44.8 g. I in 125 ml. pyridine for 10 min. gave 40% IIa (R = Bu) b5 84-5°, n20D 1.5519. Similarly IIa (R = Ph) b2.5 112-14°, n23D 1.6880 was prepared. However boiling (p-IC6H4C.tpbond.C)2Cu, with I in pyridine gave IIa (R = p-IC6H4) m. 125-30° and IIb (R = p-IC6H4) m. 245-7° (C6H6-heptane), separated by crystallization. Also (p-ClC6H4C.tpbond.C)2Cu and I gave IIa (R = p-ClC6H4C.tpbond.C) m. 80-5° and IIb (R = p-ClC6H4C.tpbond.C) m. 179-85° (heptane). To further confirm the structures of IIa and IIb they were converted to boranes by refluxing with an excess of decaborane in PhMe solution. The following were characterized (compound, % yield, and m.p. given): 1,2-bis(1-butylborenyl)ethylene, 62, 153-5° (PhMe); 1-(β -iodovinyl)-2-phenylbarene, -, 227-35° (hexane); 1-(β -iodovinyl)-2-butylbarene, -, 72-4°.

IT 10a2653-34-QP
 RL: SPW (Synthetic preparation); PRP (Properties); PREP (Preparation)
 (Interaction of diiodoethylene with copper acetylides)
 RN 10a2653-34-0 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



FILE 'HOME' ENTERED AT 10:26:39 ON 18 DEC 2009

=> file registry

=>
 Uploading C:\Program Files\STNEXP\Queries\10591950-claim 1-w 3.sr



chain nodes :
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 chain bonds :
 1-2 1-12 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-11
 exact/norm bonds :
 6-7 7-8
 exact bonds :
 1-2 1-12 2-3 3-4 4-5 5-6 8-9 9-11
 G1:Cb,Cy,Hy
 Match level :
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED
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 100.04 PROCESSED 1651 ITERATIONS 44 ANSWERS
 SEARCH TIME: 00.00.01
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 => s l3

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YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2009:1167697 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 151:470282

TITLE: Synthesis of hybrid masked triyne-phenylene axial rods containing (E)- β -chlorovinylsilanes in the π -conjugated framework

AUTHOR(S): Waller, Michael D.; Kariuki, Benson M.; Cox, Liam R.

CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK

SOURCE: Journal of Organic Chemistry (2009), 74(20), 7898-7907
CODEN: JOCEAH; ISSN: 0022-5263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Silyl-masked hexayne Me3SiC.tpbond.CC(Cl)C(SiR3)C.tpbond.CC.tpbond.C(SiR3)C.tpbond.CSiMe3 (7, SiR3 = tBuPh2Si) undergoes fluoride-induced β -elimination yielding, after terminal modifications, 1,12-diaryldodecahexaynes; compared to its positional isomer Me3SiC.tpbond.C(SiR3)C.tpbond.CC.tpbond.CC(Cl)C(SiR3)C.tpbond.CSiMe3 3 (2, same SiR3), prepared earlier, the compound 7 provides increased flexibility, allowing introduction of aromatic spacer groups, useful in production of carbyne-type mol. wires. A two-directional synthesis of a masked hexayne 7, in which two β -chlorovinylsilanes protect two of the internal alkynes, is reported. The key step involves the Pd-catalyzed oxidative dimerization of alkyne HC.tpbond.C(SiR3)C.tpbond.CC(CHE2OTHP) (10) to provide diyne TPOCE2C(Cl)C(SiR3)C.tpbond.CC.tpbond.CC.tpbond.CC(CHE2OTHP) (12), which is elaborated into centrocyn. masked hexayne 7 in four steps. Masked hexayne 7 is a constitutional isomer of masked hexayne 2, which has been used as a monomer unit for oligoyne assembly. Although masked hexayne 7 was not as convenient a building block as 2 for application in oligoyne assembly, one of its precursors, namely alkyne 10, could be used successfully in Sonogashira couplings, which allowed the incorporation of aromatic spacers and the formation of hybrid masked triyne-phenylenes Me3SiC.tpbond.CC(Cl)C(SiR3)C.tpbond.C-1,4-C6H4C.tpbond.CC(SiR3)C.tpbond.CC(CHE2OTHP) (20) and Me3SiC.tpbond.CC(Cl)C(SiR3)C.tpbond.C-1,4-C6H4C.tpbond.C(CHE2OTHP) (28). Comps. 20 and 28 both contain removable end-groups, which will permit their application as building blocks for the assembly of classes of long-chain, π -conjugated rod-like mols. Rod-like mol.

Me2C(OH)C.tpbond.CC(Cl)C(SiR3)C.tpbond.CC6H4C.tpbond.C(CHE2OTHP)C.tpbond.CC(CHE2OTHP) (34, CH4 = 1,4-phenylene), which possesses a similar conjugated scaffold as 28, was also prepared by using a similar strategy. Treatment of 34 with TBAF effected a 2-fold dechlorosilylation to provide a rigid rod mol. Me2C(OH)C.tpbond.C(CHE2OTHP)C.tpbond.C(CHE2OTHP)C.tpbond.C(CHE2OTHP)C.tpbond.C(CHE2OTHP) (35) in which two 1,4-phenylene units interrupt an octayne scaffold. IT 131:093-35-2P 1191:093-44-3P

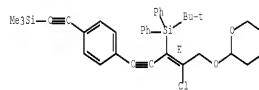
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of π -conjugated p-phenylene-bridged β -chloro silyl-substituted enynes as precursors for arylene-containing polyene mol. wires)

RN 1191093-35-2 CAPLUS

CN 2H-Pyran, 2-((1,2-bis(2-chloro-3-((1,1-dimethylethyl)diphenylsilyl)-5-[[4-(2-(trimethylsilyl)ethynyl)phenyl]-2-penten-4-yn-1-yl]oxy]tetrahydro-

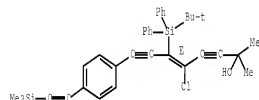
Double bond geometry as shown.



RN 1191093-44-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306161

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PFXKX2

DOCUMENT TYPE: Patent

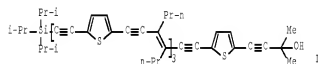
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NO 2005085176	A1	20050915	NO 2005-JP3350	20050308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BG, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GF, GR, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PE, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BM, GE, GM, KE, LS, MW, MY, NA, SD, SI, SZ, TG, UG, ZM, ZW, AM, AG, BY, BG, KD, MD, RU, TJ, TM, AT, BE, BG, CH, CI, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML,				

MR, NE, SW, TD, TG
 US 20070176164 A1 20070802 US 2007-591950 20070307
 PRIORITY APPN. INFO.: JP 2004-65446 A 20040309
 WO 2005-03950 W 20050308
 ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSIUS DISPLAY FORMAT
 OTHER SOURCE(S): MARPAT 143306181
 GI



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound 1 was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-69-7P 740810-60-0P 740810-64-4P
 740810-63-5E 740810-67-7P 740810-68-0P
 666661-71-4P 666664-00-4P 666664-04-4P
 666664-05-7P 666664-01-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

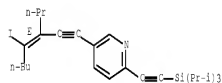
(Intermediate; preparation of π -conjugated aromatic ring-containing

acetylene derivs. as organic electroluminescent devices)

RN 740810-59-7 CAPLUS

CN Pyridine, 5-[(3S)-4-iodo-3-propyl-3-octen-1-yn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

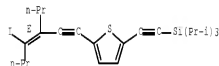
Double bond geometry as shown.



RN 740810-60-0 CAPLUS

CN Thiophene, 2-[(3S)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

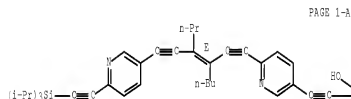
Double bond geometry as shown.



RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3S)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



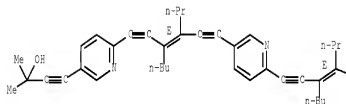
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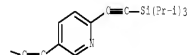
RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3S)-3-butyl-4-[2-[6-[(3S)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



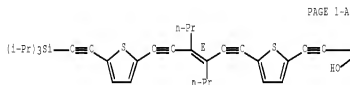
PAGE 1-A



PAGE 1-B

RN 740810-67-7 CAPLUS
 CN 3-Butyn-2-ol, 2-methyl-4-{5-[(3E)-3-propyl-4-[(5-{[tris(1-methylethyl)silyl]ethynyl}-2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl}- (CA INDEX NAME)

Double bond geometry as shown.

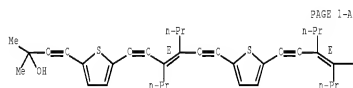


PAGE 1-B

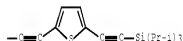


RN 740810-68-8 CAPLUS
 CN 3-Butyn-2-ol, 2-methyl-4-{5-[(3E)-3-propyl-4-[(5-{[tris(1-methylethyl)silyl]ethynyl}-2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl}ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl}- (CA INDEX NAME)

Double bond geometry as shown.

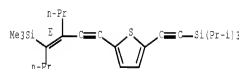


PAGE 1-B



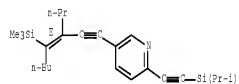
RN 864684-95-4 CAPLUS
 CN Thiophene, 2-[(3E)-3-propyl-4-(trimethylsilyl)-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



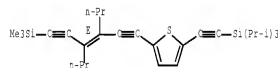
RN 864684-00-4 CAPLUS
 CN Pyridine, 5-[(3E)-3-propyl-4-(trimethylsilyl)-3-octen-1-yn-1-yl]-2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



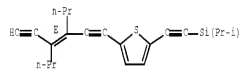
RN 864684-04-8 CAPLUS
 CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-05-9 CAPLUS
 CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

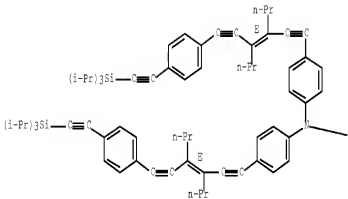
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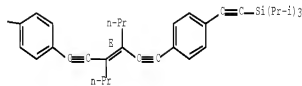
RN 864684-31-1 CAPLUS
 CN Benzenamine, N-(4-[(3E)-3,4-dipropyl-6-(4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl)-3-hexene-1,5-diyn-1-yl]phenyl)-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

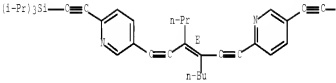


IT 740810-66-6P 740810-63-9P 866684-06-4P
866684-21-1P 866684-22-0P 866684-23-1P
866684-24-2P 866684-25-3P 866684-26-4P
866684-27-5P 866684-28-6P 866684-29-7P
866684-30-8P
RU: DEV (Device component use); IMF (Industrial manufacture); SPN
(Synthetic preparation); TEM (Technical or engineered material use); PREP
(Preparation); USES (Uses)
(preparation of *m*-conjugated aromatic ring-containing acetylene derivs. as
organic electroluminescent devices)

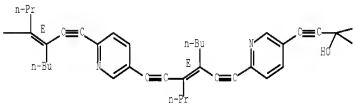
RN 740810-66-6 CAPLUS
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-
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pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX
NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



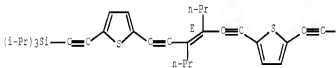
PAGE 1-C

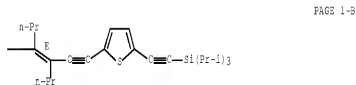
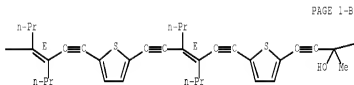


RN 740810-69-9 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-
propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-
penter-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penter-1-yn-1-yl]-2-
thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA
INDEX NAME)

Double bond geometry as shown.

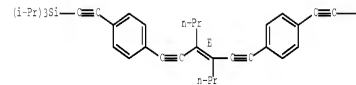
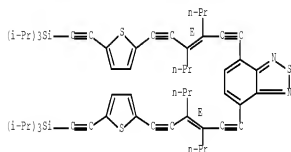
PAGE 1-A





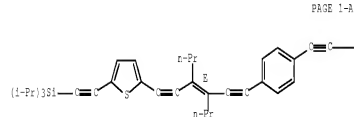
RN 864684-06-0 CAPLUS
 CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



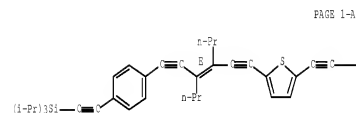
RN 864684-21-9 CAPLUS
 CN Thiophane, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

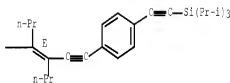
Double bond geometry as shown.



RN 864684-23-1 CAPLUS
 CN Thiophane, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



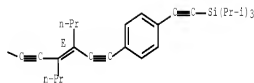


PAGE 1-B

RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynadiyl]]bis[tris(1-methylethyl)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

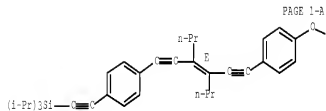


PAGE 1-B

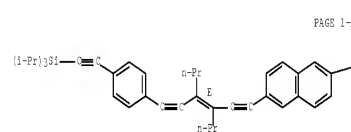
RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyne-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

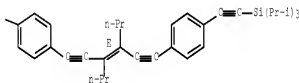
Double bond geometry as shown.



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PAGE 1-A

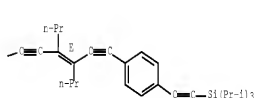


PAGE 1-B

RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyne-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

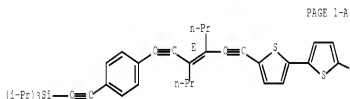


PAGE 1-B

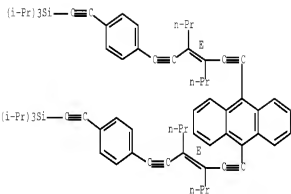
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyne-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



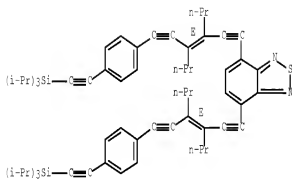
PAGE 1-A



RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

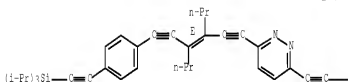
Double bond geometry as shown.



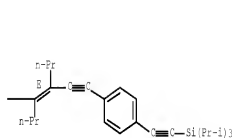
RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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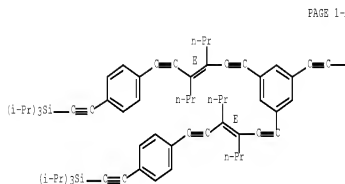


PAGE 1-B

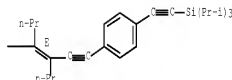
RN 864684-30-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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IT 740810-57-5

RL: RCT (Reactant); RACT (Reactant or reagent)

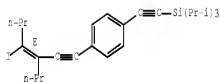
(preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic

electroluminescent devices)

RN 740810-57-5 CAPLUS

CN Benzene, 1-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-4-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

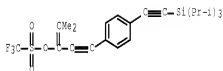
L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2005:509432 CAPLUS Full-text
 DOCUMENT NUMBER: 143:7446
 TITLE: Synthesis and characterization of cross-conjugated oligo(phenylene enynylene)s
 AUTHOR(S): Cho, Jeon; Zhao, Yuming; Tykinski, Rik R.
 CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (4), 142-150
 CODEN: ARKIVAR
 URL: http://www.arkat-usa.org/ark:/journal/2005/104_Zefirov/1369/1369.pdf

PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:7446

AB The synthesis and characterization of a series of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira protocol is reported. The structural properties of these oligomers have been established by ¹H and ¹³C NMR and IR spectroscopies, as well as mass spectrometry. Their electronic absorption and emission behavior has been investigated via UV/Vis and fluorescence spectroscopy. The results of this study demonstrate that electronic communication along the conjugated framework of these oligomers is limited due to the presence of a cross-conjugated enyne framework and arylene fragments.

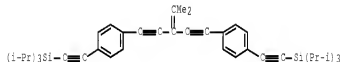
IT 452459-93-7P 852453-85-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira reaction)

RN 852459-93-7 CAPLUS
 CN Methanesulfonic acid, 1,1,1-trifluoro-, 2-methyl-1-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-1-propen-1-yl ester (CA INDEX NAME)



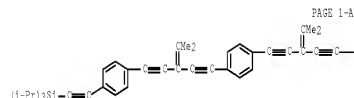
RN 852459-85-9 CAPLUS

CN Benzene, 1-[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-4-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

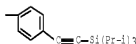


IT 452459-86-0P 852453-87-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira reaction)

RN 852459-86-0 CAPLUS
 CN Benzene, 1,4-bis[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)

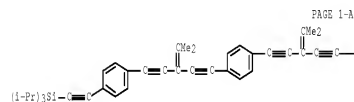


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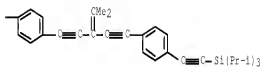
PAGE 1-B

RN 852459-87-1 CAPLUS
 CN Benzene, 1-[4-methyl-3-[2-[4-[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-4-[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)



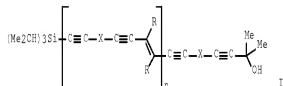
PAGE 1-A

PAGE 1-B



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STM
 ACCESSION NUMBER: 2004:490115 CAPLUS Full-text
 DOCUMENT NUMBER: 141:190674
 TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission
 AUTHOR(S): Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie
 CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan
 SOURCE: Organic Letters (2004), 6(14), 2373-2376
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:190674
 GI



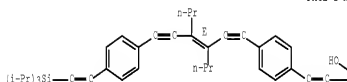
AB Synthesis and fluorescence properties of π -conjugated compds. 1 ($n = 1 - 3$; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroar. ring and an enediyne unit in the backbone are described.

IT 74/0110-61-1E 740810-60-2P 740810-60-4P
 740810-65-5P 740810-67-7E 740810-68-4P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PRP (Preparation); RACT (Reactant or reagent)

(preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the

backbone)
 RN 740810-61-1 CAPLUS
 CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-(4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



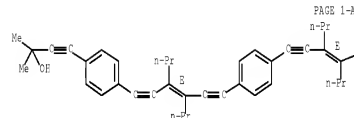
PAGE 1-A



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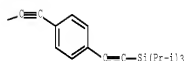
RN 740810-62-2 CAPLUS
 CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[4-[(3E)-3-propyl-4-[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



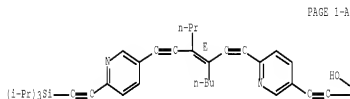
PAGE 1-A

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RN 740810-64-4 CAPLUS
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

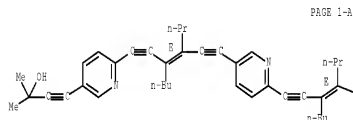


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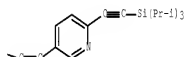


RN 740810-65-5 CAPLUS
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

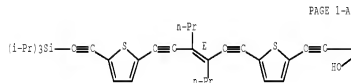


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RN 740810-67-7 CAPLUS
 CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[5-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

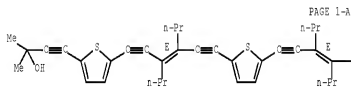


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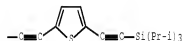


RN 740810-68-8 CAPLUS
 CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[5-[(3E)-3-propyl-4-[5-[5-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



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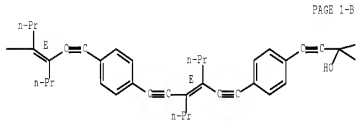
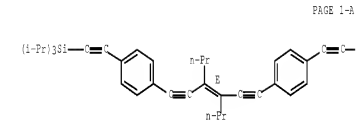


IT 740810-69-3P 740810-69-6P 740810-69-9P
 RL: PREP (Properties); SPW (Synthetic preparation); PREP (Preparation)
 (preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-63-3 CAPLUS

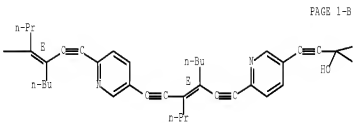
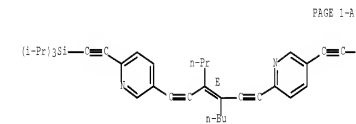
CN 3-Butyn-2-ol, 2-methyl-4-([3E]-3-propyl-4-([4-([3E]-3-propyl-4-([4-([3E]-3-propyl-4-([4-([tris(1-methylethyl)silyl)ethynyl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]phenyl)- (CA INDEX NAME)

Double bond geometry as shown.



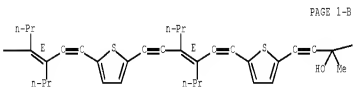
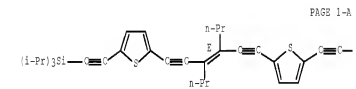
RN 740810-66-6 CAPLUS
CN 3-Butyn-2-ol, 4-[6-([3E]-3-butyl-4-[2-[6-([3E]-3-butyl-4-[2-[6-([3E]-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl)ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 740810-69-9 CAPLUS
CN 3-Butyn-2-ol, 4-[5-([3E]-4-[2-[5-([3E]-5-ethyl-4-[2-[5-([3E]-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl)ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

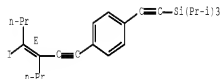
Double bond geometry as shown.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

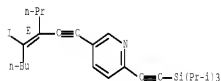
IT 740810-57-54 740810-57-7P 740810-60-02
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)
 RN 740810-57-5 CAPLUS
 CN Benzene, 1-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-4-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



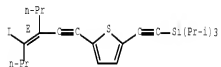
RN 740810-59-7 CAPLUS
 CN Pyridine, 5-[(3E)-4-iodo-3-propyl-3-octen-1-yn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



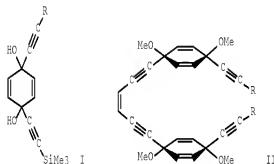
RN 740810-60-0 CAPLUS
 CN Thiophene, 2-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS

14 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2003:491916 CAPLUS Full-text
 DOCUMENT NUMBER: 139:395637
 TITLE: Synthesis of differentially protected/functionalised acetylenic building blocks from p-benzoquinone and their use in the synthesis of new enediyne
 AUTHOR(S): Sankaraman, Sethuraman; Srinivasan, Manivannan
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology Madras, Madras, 600 036, India
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(13), 2388-2392
 CODEN: OBCRAK; ISSN: 1477-0520
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:395637
 GI



AB Sequential addition of two different lithium acetylides to p-benzoquinone yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4-diols I [R = (Me₂CH)Si, (EtO)CCH] with different protective/functional groups on the two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with (Z)-1,2-dichloroethene yielded new enediyne II bearing cyclohexa-2,5-diene units.

IT 626235-20-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of cyclohexadienyl enediyne via double addition of functionalised lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethene)
 RN 626235-20-9 CAPLUS
 CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis[(cis-1,4-dimethoxy-2,5-cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 381173-15-59

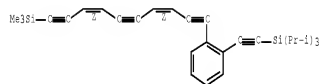
RL: PREP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 381173-15-5 CAPLUS

CN Benzene, 1-[(3Z,7E)-10-(trimethylethyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-(tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 381173-15-59

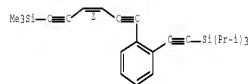
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 381173-13-3 CAPLUS

CN Benzene, 1-[(3Z)-6-(trimethylethyl)-3-hexene-1,5-diyn-1-yl]-2-[2-(tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

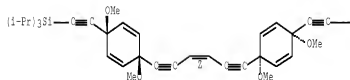


OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (33 CITINGS)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN

PAGE 1-A



PAGE 1-B

—Si(Pr-1)3

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2002:074017 CAPLUS Full-text

DOCUMENT NUMBER: 138:7C938

TITLE: Diatropicity of 3,4,7,8,9,10,13,14-Octadehydro[14]annulenes: A Combined Experimental and Theoretical Investigation
AUTHOR(S): Boydston, Andrew J.; Haley, Michael M.; Williams, Richard Vaughan; Armantrout, John R.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Journal of Organic Chemistry (2002), 67(25), 8812-8919
CODEN: JOCEAH; ISSN: 0022-5263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:7C938

AB The synthesis and study of a series of octadehydro[14]annulenes is described. The aromaticity of these annulenes was investigated through examination of exptl. data from arene-fused systems as well as calculated nucleus-independent chemical shifts (NICS) and bond lengths. Benzene ring fusion to the parent system results in a stepwise loss in aromaticity as the number of fused rings is increased from one to two to three. This decrease in annulenic ring current is manifested in the alkene proton chemical shifts (0-2 benzenes) as well as the NICS (0-3 benzenes). Comparison of isomeric thiophene-fused annulenes shows further evidence of ring current competition as these allow for observation of intermittent degrees of delocalization throughout the annulenic core. A consistent relationship between the magnitude of the NICS values and the degree of benzannulation is also observed

IT 482234-13-39

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cross-coupling; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482234-13-9 CAPLUS

CN Benzene, 1-(3Z)-3-hexene-1,5-diyn-1-yl-2-[2-(tris(1-

ACCESSION NUMBER: 2001:731976 CAPLUS Pull-text
 DOCUMENT NUMBER: 136:53492
 TITLE: Diatropicity of Dehydrobenzo[14]annulenes: Comparative Analysis of the Bond-Fixing Ability of Benzene on the Parent 3,4,7,8,9,10,13,14-Octadehydro[14]annulene
 AUTHOR(S): Boydston, A. J.; Haley, Michael M.
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA
 SOURCE: Organic Letters (2001), 3(22), 3599-3601
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:53492

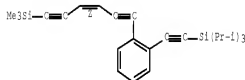
AB We report the synthesis of 3,4,7,8,9,10,13,14-octadehydro[14]annulene and detail a comparative aromaticity study with its benzannelated derivs. (e.g., benzo[e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene and dibenzo[a,e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene).

IT 381173-13-38 381173-15-39
 RI: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (intermediate; diatropicity of dehydrobenzoannulenes)

RN 381173-13-3 CAPLUS

CN Benzene, 1-[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

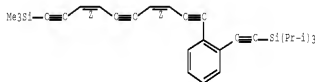
Double bond geometry as shown.



RN 381173-15-5 CAPLUS

CN Benzene, 1-[(3Z,7Z)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

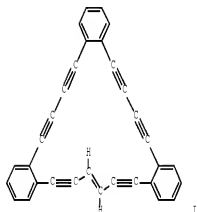


OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2001:714296 CAPLUS Pull-text
 DOCUMENT NUMBER: 136:69640

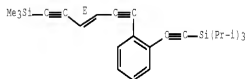
TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units
 AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.
 CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA
 SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490
 CODEN: EJOCFY; ISSN: 1434-193X
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:69640
 GI



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzylation.

IT 214628-16-14 214628-17-39 214628-18-39
 361004-08-45
 RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)
 RN 214628-16-7 CAPLUS
 CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

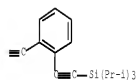


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RN 214628-17-8 CAPLUS

CN Silane, tris(1-methylethyl)[(2-[(3E)-6-(2-[4-(2-[(tris(1-methylethyl)silyl]ethynyl]phenyl)-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl)- (3CI) (CA INDEX NAME)

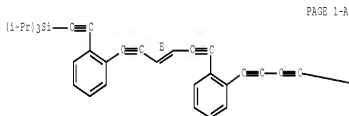
Double bond geometry as shown.



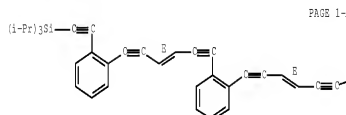
RN 383404-38-4 CAPLUS

CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (3CI) (CA INDEX NAME)

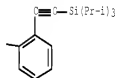
Double bond geometry as shown.



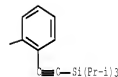
PAGE 1-A



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PAGE 1-B



PAGE 1-B

RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[(2-[6-(2-[(3E)-6-(2-[(tris(1-methylethyl)silyl]ethynyl]phenyl)-3-hexene-1,5-diynyl]phenyl)-1,3,5-hexatriynyl]phenyl]ethynyl)- (3CI) (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2000:832492 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 134:310920

TITLE: Bis(enediynes) Macrocycles: Synthesis, Reactivity, and Structural Analysis

AUTHOR(S): Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.

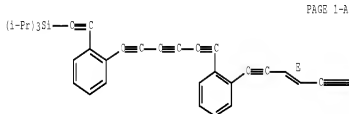
CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Tetrahedron (2000), 56(49), 9581-9588

CODEN: TETNAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal



PAGE 1-A

LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:310920

AB The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediyne) comps. The solid-state packing of one of the comps. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization

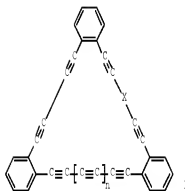
IT 335378-20-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

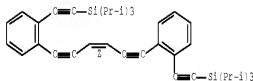
(preparation of bis(enediyne) macrocycles)

RN 335378-20-6 CAPLUS

CN Silane, [(3E)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)



Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 1998:606810 CAPLUS Full-text

DOCUMENT NUMBER: 129:302407

ORIGINAL REFERENCE NO.: 129:61683a,61686a

TITLE: Synthesis of expanded planar dehydrobenzoannelenes: weakly diatropic, weakly paratropic, or atropic?

AUTHOR(S): War, W. Brad; Kimball, David S.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA

SOURCE: Tetrahedron Letters (1998), 39(38), 6795-6798

CODEN: TETLEA; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:302407

GI

AB Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannelenes **1** [X = C,sp.bond.C, (E)-CH=CH; n = 0,1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannulation, dehydrobenzoannelenes possess weak induced ring currents.

IT 214628-16-7P 214623-17-8P 214628-18-9P

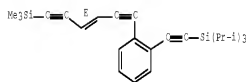
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of expanded planar dehydrobenzoannelenes with triacetylenic linkages)

RN 214628-16-7 CAPLUS

CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

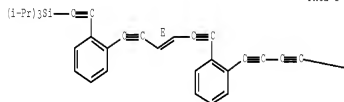
Double bond geometry as shown.



RN 214628-17-8 CAPLUS

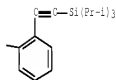
CN Silane, tris(1-methylethyl)[(2-[(3E)-6-(2-(4-[tris(1-methylethyl)silyl]ethynyl)phenyl]-1,3-butadiynyl)phenyl]-3-hexene-1,5-diynyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



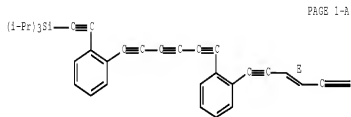
PAGE 1-A

PAGE 1-B



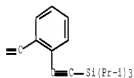
RN 214628-18-9 CAPLUS
CN Silane, tris(1-methylethyl)[(2-{6-[2-[(3E)-6-[2-[(tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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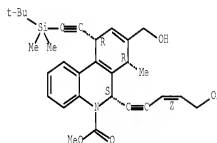


OS.CITING REF COUNT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 1997:474343 CAPLUS Full-text
DOCUMENT NUMBER: 127:161614
ORIGINAL REFERENCE NO.: 127:31327a,31330a
TITLE: A new approach to a dynemicin A analog by using an intramolecular Diels-Alder reaction
AUTHOR(S): Sakamoto, Yasuharu; Takahashi, Takashi
CORPORATE SOURCE: Dep. Chem. Eng., Tokyo Inst. Technol., Tokyo, 152, Japan
SOURCE: Synlett (1995), (Spec. Issue), 513-515

PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:161614
AB New synthetic approach to the dynemicin skeleton by using an intramol. Diels-Alder reaction and its diastereoselectivity based on an "TM2 transition-state model" are described.
IT 193999-00-5P
RI: SPW (Synthetic preparation); PREP (Preparation)
(synthesis of a dynemicin A analog by using an intramol. Diels-Alder reaction)
RN 193688-00-5 CAPLUS
CN 5 (6R)-Phenanthridinecarboxylic acid, 10-[2-[(1,1-dimethylethyl)dimethylsilyl]ethynyl]-7,10-dihydro-8-(hydroxymethyl)-6-[(3E)-5-hydroxy-3-penten-1-yn-1-yl]-7-methyl-, methyl ester, (6R,7S,10S)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 chain bonds :
 1-2 1-9 2-3 3-4 4-5 5-6 6-7
 exact/norm bonds :
 1-9 4-5 5-6
 exact bonds :
 1-2 2-3 3-4 6-7

GI:Cb,Cy,HY

Match level :
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS

L1 STRUCTURE UPLOADED

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 SAMPLE SCREEN SEARCH COMPLETED - 623 TO ITERATE

100.04 PROCESSED 623 ITERATIONS 2 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 10963 TO 13957
 PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

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 FULL SCREEN SEARCH COMPLETED - 11729 TO ITERATE

100.04 PROCESSED 11729 ITERATIONS 53 ANSWERS
 SEARCH TIME: 00.00.01

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 C
 => s l3
 L4 20 L3

=> G ibib abs hitstr 1-
 YOU HAVE REQUESTED DATA FROM 20 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2009:76616 CAPLUS [full-text](#)
 DOCUMENT NUMBER: 150:167710
 TITLE: Push-pull hyperbranched molecules. A theoretical study
 AUTHOR(S): Ramos, Estrella; Guadarrama, Patricia; Teran, Gerardo;
 Fomine, Serguei
 CORPORATE SOURCE: Instituto de Investigaciones en Materiales,
 Universidad Nacional Autonoma de Mexico, Mexico,

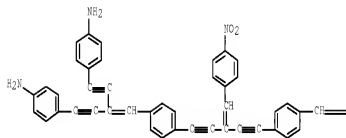
SOURCE: 04510, Mex.
 Journal of Physical Organic Chemistry (2009), 22(1),
 9-16
 CODEN: JPOCEE; ISSN: 0894-3230
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The electronic properties of the ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups have been studied at B3LYP/cc-pvtz//HF/6-31g(d), TD-B3LYP/cc-pvtz//HF/6-31g(d) and TD-B3LYP/cc-pvtz//CIS/6-31g(d) levels of theory, resp. It was demonstrated that dendritic architecture of push-pull mols. favors the charge transfer in the excited state compared to linear mols. The possibility of adopting a plane conformation is an important condition for the charge transfer in an excited state. According to the calcs. 1:1 ratio of donor and acceptor groups is another important precondition for the manifestation of strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the S0 -> S1 transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

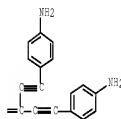
IT 1107616-31-6 1107616-72-7 1107616-33-8
 RI: PRP (Properties)
 (electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

RN 1107616-71-6 CAPLUS
 CN Benzenamine, 4,4'-[3-[[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-nitrophenyl)methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

PAGE 1-A



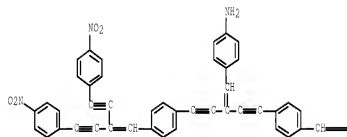
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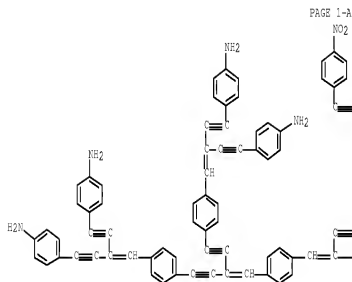
RN 1107616-72-7 CAPLUS

CN Benzenamine, 4,4'-[3-[[4-[5-[4-(4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-[4-[4-(4-nitropheryl)-2-[2-(4-nitropheryl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[4-[4-(4-nitropheryl)-2-[2-(4-nitropheryl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

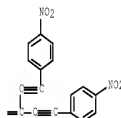
PAGE 1-A



PAGE 1-A



PAGE 1-B



IT 1107616-16-1

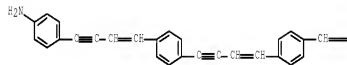
RL: FRP (Properties)

(linear analog; electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

RN 1107616-16-1 CAPLUS

CN Benzenamine, 4-[[4-[[4-[[4-[[4-[[4-(4-nitropheryl)-1-buten-3-yn-1-yl]phenyl]-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

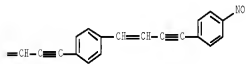
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RN 1107616-13-8 CAPLUS

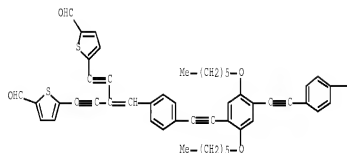
CN Benzenamine, 4-[[4-[[4-[[4-[[4-[[4-(4-nitropheryl)-2-[2-(4-nitropheryl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-[[4-[[4-[[4-[[4-(4-nitropheryl)-2-[2-(4-nitropheryl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

PAGE 1-B



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2008:355050 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 148:520471
 TITLE: Tetrafullerene Conjugates for All-Organic Photovoltaics
 AUTHOR(S): Fernandez, Gustavo; Sanchez, Luis; Veldman, Dirk; Wienk, Martin M.; Atienza, Carmen; Guldi, Dirk M.; Janssen, Rene A. J.; Martin, Nazario
 CORPORATE SOURCE: Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Madrid, 28040, Spain
 SOURCE: Journal of Organic Chemistry (2008), 73(8), 3189-3196
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 148:520471

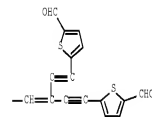


AB The synthesis of two new tetrafullerene nanocomposites in which four C60 units are covalently connected through different π -conjugated oligomers (oligo(p-phenylene ethynylene) and oligo(p-phenylene vinylene)) is described. The photovoltaic response of these C60-based conjugates was evaluated by using them as the only active material in organic solar cells, showing a low photovoltaic performance. Photophys. studies in solution demonstrated a very fast (.apprx.10 ps) deactivation of the singlet excited state of the central core unit to produce both charge-separated species (i.e., C60^{•-}-oligomer^{•+} (C60)3 and C60 centered singlet excited states). The charge-separated state recombines partly to the C60 centered singlet state that undergoes subsequent intersystem crossing. Photophys. studies carried out in films support these data, exhibiting long-lived triplet excited states. For both tetrafullerene arrays, the low yield of long-lived charge carriers in thin films accounts for the limited photovoltaic response. On the contrary, utilizing the oligo(p-phenylene vinylene) centered precursor aldehyde as an electron donor and antennae unit and mixing with the well-known C60 derivative PCBM, the photophys. studies in films show the formation of long-lived charges. The photovoltaic devices constructed from these mixts. showed a relatively high photocurrent of 2 mA/cm². The sharp contrast between the nanocomposites and the phys. blends tentatively was attributed to improved charge dissociation and the collection of more favorable energy levels in the blends as a result of partial aggregation of both of the components.

IT 1022991-37-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PRP (Preparation); RACT (Reactant or reagent)

(In synthesis of tetrafullerene conjugates for all-organic photovoltaics)

RN 1022991-37-2 CAPLUS
 CN 2-Thiophenecarboxaldehyde, 5,5'-[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-(2-(5-formyl-2-thienyl)ethynyl)-3-butan-1-yn-4,1-diyl]]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2008:244421 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 148:403337
 TITLE: Triphenylphosphine Incorporation Reactions of Diynyl Complexes Containing a TpRu(NO) Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene
 AUTHOR(S): Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Kenta; Umakoshi, Katsuke; Onishi, Masayoshi
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan
 SOURCE: Organometallics (2008), 27(6), 1227-1233
 CODEN: ORGNM7; ISSN: 0276-7333
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 148:403337

AB Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand (Tp = B[pyrazol-1-yl]3) were prepared, and their reactivities toward PPh3 incorporation in the presence of HBF4·Et2O were described. The PPh3 incorporation of mono(arylbutadiynyl) complex TpRuCl(C(C.tpbond.C-C.tpbond.C-CtHMe)(NO) (1) resulted in the β -phosphonolalkenyl complex (5) -

[TpRuCl(CH₃C(PPh₃)-C.tpbond.C- C6H4Me)(NO)]BF₄ (2-BF₄), whereas when bis(arylbutediynyl) TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)2(NO) (3) was treated, mono- and bis(β-phosphonoalkenyl) complexes E)-[TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)(CH₃C(PPh₃)-C.tpbond.C- C6H4Me)(NO)]BF₄ (4-BF₄) and E,E)-[TpRu(CH₃C(PPh₃)-C.tpbond.C-C6H4Me)2(NO)]BF₄2 (5-BF₄)2 were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutediynyl) (3-hydroxyalkenyl) complex, TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)(C.tpbond.CCPH2(OH))(NO) (6), was allowed to react with PPh₃ in the presence of the protic acid to give the α-phosphonoalkenyl [TpRu(C.tpbond.C-C.tpbond.C- C6H4Me)(C(PPh₃);C:CPH2)(NO)]BF₄ (7-BF₄). Interestingly, thermal isomerization of 7-BF₄ to a ruthena-2-PPh₃-cyclobuta[b]naphthalene [TpRu(CH(PPh₃)[3-Ph-8-(MeC6H4-C.tpbond.C- ClOH4)](NO)]BF₄ (8-BF₄) was observed

IT 1015477-27-66

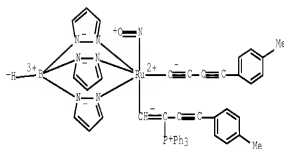
RL: SPW (Synthetic preparation); PREP (Preparation)
(triphenylphosphine incorporation reactions of diynyl complexes containing pyrazolylboratoruthenium nitrosyl fragment and isomerization to ruthenacyclobutanaphthalene)

RN 1015477-27-6 CAPLUS

CN Ruthenium(1+), [hyocitris(1β-pyrazolato-κN)]borato(1-)-κN2,κN2',κN2''[4-(4-methylphenyl)-1,3-butadiyn-1-yl] [(1E)-4-(4-methylphenyl)-2-(triphenylphosphonio)-1-buten-3-yn-1-yl]nitrosyl, (OC-6-24)-, tetrafluoroborate(1-)(1:1) (CA INDEX NAME)

CM 1

CRN 1015477-26-5
CMF C49 H40 B N7 O P Ru
CCI CCS



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

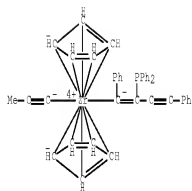
14 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 20071105060 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 148:11306
TITLE: Formation and Structural and Dynamic Features of Atropisomeric η²-Iminoacyl Zirconium Complexes
AUTHOR(S): Spies, Patrick; Kehr, Gerald; Kehr, Seda; Froehlich, Roland; Eriker, Gerhard
CORPORATE SOURCE: Organisch-Chemisches Institut, Universitaet Muenster, Muenster, 48149, Germany
SOURCE: Organometallics (2007), 26(23), 5612-5620
CODEN: ORGNMT; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:11306
AB The Cp₂ZrCl(CPh)(C(X)2.C.tpbond.CPh) complexes 7a (X = Ph) and 10 (X = C6F5) insert tert-butylisonitrile into the Zr-C(sp²) σ bond to yield the iminoacyl zirconocene complexes, Cp₂ZrCl(C(H)OMe)(CPh)(C(X)2.C.tpbond.CPh) 13a and 13b. X-ray crystal structure anal. of complexes 13a and 13b revealed a chiral atropisomeric structure with a torsion angle of 74.6(2)° (13a) and 72.9(6)° (13b), resp., around the central iminoacyl/alkenyl C(sp²)-C(sp²) σ bond. In solution an analogous chiral structure is observed. The barrier of interconversion of the enantiomeric atropisomers of 13a and 13b was determined at ΔG_{thermod.} (327K) = 14.9 ± 0.3 kcal mol⁻¹ (13a) and ΔG_{thermod.} (325K) = 14.8 ± 0.3 kcal mol⁻¹ (13b) by temperature-dependent dynamic NMR spectroscopy. Reaction of 7a and 10 with methylolithium followed by treatment with B(C6F5)₃ gave the corresponding cationic zirconocene complexes Cp₂Zr⁺(THF)(CPh)(C(X)2.C.tpbond.CPh) [MeB-(C6F5)₃] 12a and 12b. These complexes took up 2 mol equiv of tert-butylisonitrile to yield the cationic η²-iminoacyl zirconocene systems 14a and 14b as isonitrile adducts. The cationic complexes 14a and 14b are also axially chiral. The barriers of enantiointerconversion (ΔG_{thermod.} (288 K) = 13.1 ± 0.3 kcal mol⁻¹ (14a), ΔG_{thermod.} (293 K) = 13.4 ± 0.3 kcal mol⁻¹ (14b)) were also determined by dynamic NMR spectroscopy.

IT 559453-54-5p

RL: PRP (Properties); SPW (Synthetic preparation); PREP (Preparation)
(crystal structure; isonitrile insertion reaction into neutral and cationic butenynylzirconocene complexes to give atropisomeric iminoacyl zirconocene complexes)

RN 958635-66-0 CAPLUS

CN Zirconium, bis[η⁵-2,4-cyclopentadien-1-yl] [(1E)-2-(diphenylphosphino)-1,4-diphenyl-1-buten-3-yn-1-yl]-1-propyn-1-yl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2007:995140 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:448227

TITLE: Convenient synthesis of (1-propynyl)arenes through a one-pot double elimination reaction, and their conversion to enynes

AUTHOR(S): An, De-Lie; Zhang, Zhiyang; Orita, Akihiro; Mineyama, Hidetaka; Otera, Junzo

CORPORATE SOURCE: Department of Chemistry, College of Chemistry and Chemical Engineering, Hunan University, Changsha, 410082, Peop. Rep. China

SOURCE: Synlett (2007), (12), 1909-1912

CODEN: SYNL5; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:448227

AB A series of prop-1-ynyl arenes were prepared by one-pot double elimination reaction of 2-benzyloxy, aromatic aldehyde, and ClPO(OEt)₂ in THF with a base such as BuLi and t-BuOK. A propargyllithium, which was prepared by treatment of propyn-1-yl arene with BuLi in the presence of 1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU), reacted with aromatic aldehyde, ClPO(OEt)₂ and t-BuOK to afford 4-arylbut-3-en-1-ynyl arene. Photoluminescence of the enynes thus prepared was recorded both in solution and in the solid state.

IT 95:766-78-09

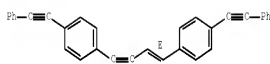
RL: SPW (Synthetic preparation); PREP (Preparation)

(preparation of propynyl arenes through one-pot double elimination and conversion to enynes)

RN 95:766-78-2 CAPLUS

CN Benzene, 1,1'-(1E)-1-buten-3-yno-1,4-diylbis[4-(2-phenylethynyl)]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2006:82014 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:334159

TITLE: Light harvesting tetrafullerene nanorearray for organic solar cells

AUTHOR(S): Atienza, Carmen M.; Fernandez, Gustavo; Sanchez, Luis; Martin, Mazarlo; Dantas, Ines S.; Wienk, Martijn M.; Janssen, Rene A. J.; Rahman, G. M. Ashkur; Guldi, Dirk M.

CORPORATE SOURCE: Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense, Madrid, E-28040, Spain

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (5), 514-516

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:334159

AB A light absorbing π -conjugated oligomer-tetrafullerene nanorearray was synthesized and its photophysics study reveals an intramolecular energy transfer. A photovoltaic device fabricated from this nanorearray and poly(3-hexylthiophene) shows an external quantum efficiency of 18% at 500 nm.

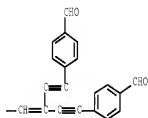
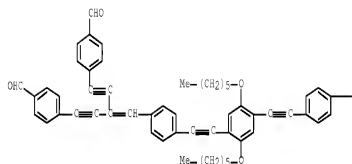
IT 880486-74-82

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PYP (Physical process); RCT (Reactant); SPW (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(compound 4; light harvesting tetrafullerene nanorearray for organic solar cells)

RN 880486-74-8 CAPLUS

CN Benzaldehyde, 4,4'-[[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl]-4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yno-4,1-diyl]]]bis- (SC1) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS
RECORD (16 CITINGS)
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2003 ACS on STM

ACCESSION NUMBER: 2005:1004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yunki

PATENT ASSIGNER(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

COGEN: PIKXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
N: AG, AG, AL, AM, AI, AU, AZ, BA, BB, BG, BN, BW, BY, BG, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, EA, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI,				

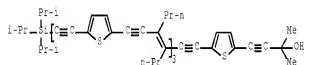
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BN: BM, GE, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, BG, KZ, MD, MG, TJ, TM, AT, BE, BG, CH, CI, CG, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, ML, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GW, HQ, ML, ME, NE, SN, TD, TG

US 20070176164 A1 20070802 US 2007-591950 20070307
PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309
WO 2005-JP3950 W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSPS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

G1



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound 1 was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 864684-11-7P 864684-12-8P 864684-13-9P

864684-15-1P 864684-16-4P 864684-17-5P

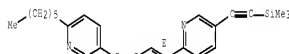
RI: IMP (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Intermediate; preparation of π -conjugated aromatic ring-containing acetylene

derivs. as organic electroluminescent devices)

RN 864684-11-7 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-(2-(trimethylsilyl)ethynyl)- (CA INDEX NAME)

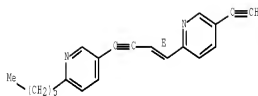
Double bond geometry as shown.



RN 864684-12-8 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

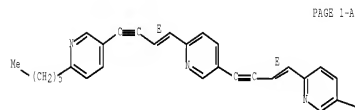
Double bond geometry as shown.



RN 864684-13-9 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[(3E)-4-[5-[2-(trimethylsilyl)ethynyl]-2-pyridinyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

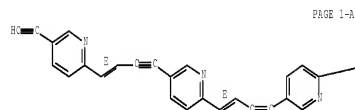
PAGE 1-B



RN 864684-15-1 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



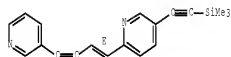
PAGE 1-A



RN 864684-18-4 CAPLUS

CN Pyridine, 2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

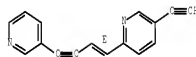
Double bond geometry as shown.



RN 864684-19-5 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 864684-16-2P 864684-17-3B 864684-20-8B

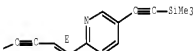
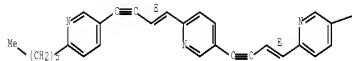
RI: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREZ (Preparation); USES (Uses)

(preparation of π-conjugated aromatic ring-containing acetylene derive. as organic electroluminescent devices)

RN 864684-16-2 CAPLUS

CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

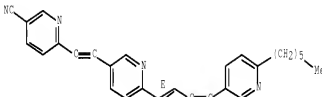
Double bond geometry as shown.



RN 864684-17-3 CAPLUS

CN 3-Pyridinecarbonitrile, 6-[2-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]ethynyl]- (CA INDEX NAME)

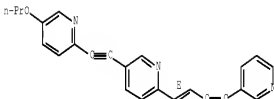
Double bond geometry as shown.



RN 864684-20-8 CAPLUS

CN Pyridine, 5-[2-(5-propoxy-2-pyridinyl)ethynyl]-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 2004:832644 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:38113

TITLE: Site-Selective Monotitanation of Dialkynylpyridines and Its Application for Preparation of Highly Fluorescent π -Conjugated Oligomers

AUTHOR(S): Takayama, Yunki; Hanazawa, Takeshi; Andou, Tomohiro; Murasaka, Kenji; Ohtani, Hiroyuki; Takahashi, Mizuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan

SOURCE: Organic Letters (2004), 6(23), 4253-4256
CODEN: ORLEF; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:38113

AB Reaction of Ti(O-*i*-Pr)₄/2i-PrMgCl reagent with 2,*n*-bis[(trimethylsilyl)ethynyl]pyridines, where *n* is 3, 4, 5, and 6, or with 3,4-bis[(trimethylsilyl)ethynyl]pyridines, proceeded with excellent site-selectivity to afford the corresponding monotitanated complex. Synthetic application of the reaction was demonstrated by an efficient preparation of π -conjugated oligomers having pyridine and arylene units alternately, which possess intense blue fluorescence emission. Thus, reaction of 2,3-bis[(trimethylsilyl)ethynyl]pyridine with Ti(O-*i*-Pr)₄/2i-PrMgCl reagent in Et₂O gave 84% (E)-2-[2-(trimethylsilyl)ethynyl]-3-[(trimethylsilyl)ethynyl]pyridine.

IT 805240-17-5P 805240-18-UP

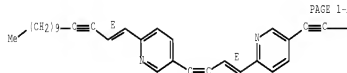
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PRP (Preparation); RACT (Reactant or reagent)

(preparation and site-selective monotitanation of dialkynylpyridines and its application for preparation of highly fluorescent π -conjugated oligomers)

RN 805240-17-9 CAPLUS

CN Pyridine, 2-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

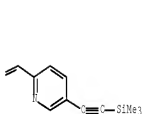
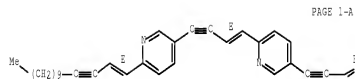
Double bond geometry as shown.



RN 805240-18-0 CAPLUS

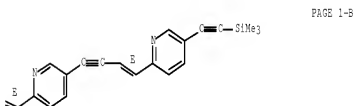
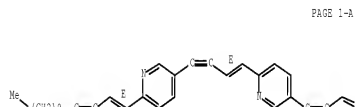
CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 805240-14-IP
 RL: PREP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and site-selective monofunctionation of dialkynylpyridines and
 its application for preparation of highly fluorescent pi-conjugated oligomers)
 RN 805240-19-1 CAPLUS
 CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-4-[6-[(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

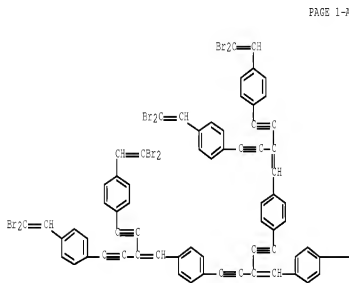
Double bond geometry as shown.

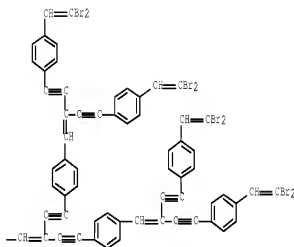


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
 (2 CITINGS)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

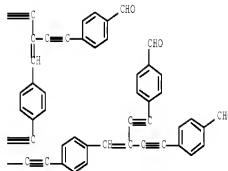
14 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2009 ACS on STW
 ACCESSION NUMBER: 2004:566840 CAPLUS Full-text
 DOCUMENT NUMBER: 141:261152
 TITLE: π -Conjugated Dendrimers Based on Bis(enediynyl)benzene Units
 AUTHOR(S): Hwang, Gil Tae; Kim, Byeang Hyeon
 CORPORATE SOURCE: National Research Laboratory, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
 SOURCE: Organic Letters (2004), 6(16), 2663-2672
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB We have synthesized a new family of π -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The comds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.
 IT 754233-15-4P 754233-19-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (convergent and divergent synthesis of π -conjugated dendrimers based on bis(enediynyl)benzene units)
 RN 754233-16-4 CAPLUS
 CN Benzene, 1,4-bis[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (3CI) (CA INDEX NAME)





RN 754233-18-6 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-[[4-[[4-(4-formylphenyl)-2-[[4-formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[[4-(4-formylphenyl)-2-[[4-formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yn-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

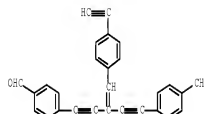
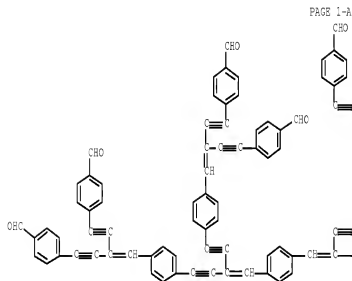


IT 206181-75-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(in convergent approach; convergent and divergent synthesis of
n-conjugated dendrimers based on bis(enediynyl)benzene units)

RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:382959 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:88772

TITLE: Electrochemical and theoretical study of a family of fully conjugated dendritic oligomers

AUTHOR(S): Osorio, Gabriela; Frontana, Carlos; Guadarrama, Patricia; Frontana-Urbe, Bernardo A.

CORPORATE SOURCE: Instituto de Química, UNAM, Circuito Exterior Ciudad Universitaria, México, 04510, Mex.
SOURCE: Journal of Physical Organic Chemistry (2004), 17(5), 439-447

CODEN: JPOCEE; ISSN: 0894-3230

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

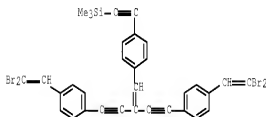
AB Novel dendritic oligomers of β,β -dibromo-4-ethynylstyrene and formyl-4-ethynylstyrene were electrochem. and theor. studied to gain a better insight into their redox behavior. Correlations between calculated ionization and exptl. oxidation potentials (arodic peak potentials) were established. The best correlation was obtained when two important effects are considered in the theor. calcns., probing their strong influence: (a) structural re-accommodation in the formed radical cation and (b) solvation effects. The effect of dendritic terminal groups (dibromovinyl and formyl groups) was also analyzed. A different redox behavior was observed for these two terminal groups, presumably due to a difference in their oxidation mechanisms. A global chemical transformation for the oxidation of dibromovinyl-terminated oligomers was proposed, providing a satisfactory explanation of the electrochem. behavior within this family of (presence of adsorptive phenomena). Taking these results into account, it is possible to explain how the cation-radical species formed in these conjugated dendritic oligomers behave when cyclic voltammetry technique is applied.

IT 716327-89-8 716327-90-1 716327-91-2

RL: CPS (Chemical process); FNU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (electrochem. and theor. study of fully conjugated dendritic oligomers family)

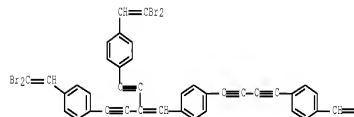
RN 716327-89-8 CAPLUS

CN Silane, [[4-[4-(4-(2,2-dibromoethenyl)phenyl)-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (3CI) (CA INDEX NAME)

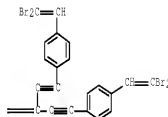


RN 716327-90-1 CAPLUS

CN Benzene, 1,1'-(1,3-butadiene-1,4-diyl)bis[4-[4-(4-(2,2-dibromoethenyl)phenyl)-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1+) (3CI) (CA INDEX NAME)



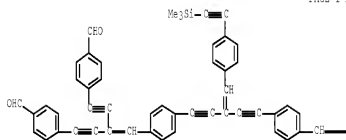
PAGE 1-A



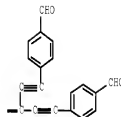
PAGE 1-B

RN 716327-91-2 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiene-1,5-diyl]bis[4,1-phenylene]3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]bis-, radical ion(1+) (3CI) (CA INDEX NAME)



PAGE 1-A



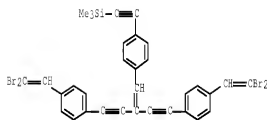
PAGE 1-B

IT 206181-72-8 206181-74-4 206181-75-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (electrochem. and theor. study of fully conjugated dendritic oligomers family)

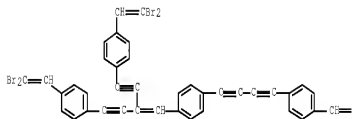
RN 206181-72-8 CAPLUS

CN Silane, [[4-[4-(4-(2,2-dibromoethenyl)phenyl)-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (3CI) (CA INDEX NAME)

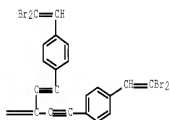


RN 206181-74-0 CAPLUS
 CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]]- (9CI) (CA INDEX NAME)

PAGE 1-A

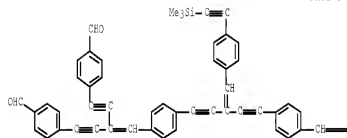


PAGE 1-B

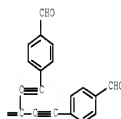


RN 206181-76-2 CAPLUS
 CN Benzaldehyde, 4,4'-[[3-[[4-[[4-(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiene-1,5-diyl]]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]]-3-buten-1-yn-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

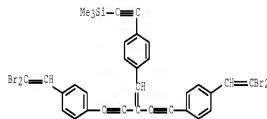
PAGE 1-A



PAGE 1-B



IT 717144-23-5 717144-24-6 717144-23-7
 RL: FMU (Formation, unclassified); FRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
 (electrochem. and theor. study of fully conjugated dendritic oligomers family)
 RN 717144-23-5 CAPLUS
 CN Silane, [[4-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1-)] (9CI) (CA INDEX NAME)



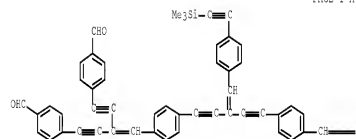
RN 717144-24-6 CAPLUS
 CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]]-, radical ion(1-)] (9CI) (CA INDEX NAME)

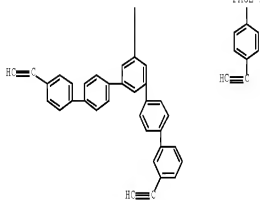
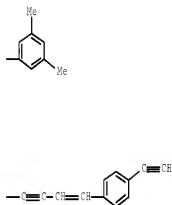
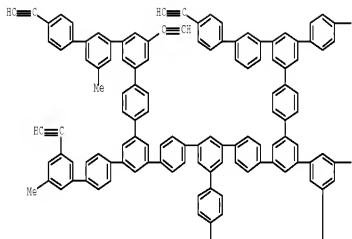
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020119612	A1	20020829	US 2001-14459	20011214
US 6576562	B2	20030610		
JP 2002305187	A	20021018	JP 2001-381504	20011214
JP 3504247	B2	20040308		

AB A manufacturing method of semiconductor device comprises (1) forming a mask material having an aromatic ring and carbon content of 2 to 8 on an object, (2) forming a mask material pattern by etching the mask material to a desired pattern, and (3) etching the object to transfer the mask material pattern: as a mask to the object.

RN 452303-35-4 CAPLUS

PAGE 1-B

O=Cc1ccc(cc1)C(=O)C#CC(=O)c2ccc(cc2)C=O

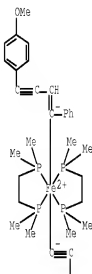


OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

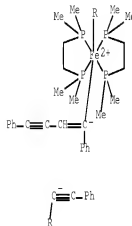
14 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:198497 CAPLUS Full-text
DOCUMENT NUMBER: 136:401857
TITLE: Acetylide-Bridged Organometallic Oligomers via the Photochemical Metathesis of Methyl-Iron(II) Complexes
AUTHOR(S): Field, Leslie D.; Turnbull, Anthony J.; Turner, Peter
CORPORATE SOURCE: School of Chemistry, The University of Sydney, Sydney, 2006, Australia
SOURCE: Journal of the American Chemical Society (2002), 124(14), 3692-3702
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:401857
AB The acetylide Me iron(II) complexes, cis/trans-[Fe(dmpe)2(C.tplbond.CR)(CH3)] (1) and trans-[Fe(depe)2(C.tplbond.CR)(CH3)] (2) [dmpe = 1,2-dimethylphosphinoethane; depe = 1,2-diethylphosphinoethane], were synthesized by transmetalation from the corresponding alkyl halide complexes. Acetylide Me iron(III) complexes were also formed by transmetalation from the chloride complexes, trans-[Fe(dmpe)2(C.tplbond.CR)(Cl)] or trans-[Fe(depe)2(C.tplbond.CR)(Cl)]. The structure of trans-[Fe(dmpe)2(C.tplbond.CO6H5)(CH3)] (1a) was determined by single-crystal x-ray diffraction. The Me acetylide iron complexes, [Fe(dmpe)2(C.tplbond.CR)(CH3)] (1), are thermally stable in the presence of acetylenes; however, under UV irradiation, methane is lost with the formation of a metal bisacetylide. Photochem. metathesis of cis- or trans-[Fe(dmpe)2(CH3)(C.tplbond.CR)] [R = CH3 (1a), 4-CH3OCH3 (1b)] with terminal acetylenes was used to selectively synthesize unsym. substituted iron(III) bisacetylide complexes of the type trans-[Fe(dmpe)2(C.tplbond.CR)(C.tplbond.CR')] [R = Ph, R' = Ph (6a), 4-CH3OC6H4 (6b), tBu (6c), SiMe3 (6d), (CH2)4C.tplbond.CR (6e); R = 4-CH3OC6H4, R' = 4-CH3OC6H4, (6g), tBu (6h), (CH2)4C.tplbond.CR (6i), adamantyl (6j)]. The structure of the unsym. iron(III) bisacetylide complex trans-[Fe(dmpe)2(C.tplbond.CO6H5)(C.tplbond.CO6H4OCH3)] (6b) was determined by single-crystal x-ray diffraction. The photochem. metathesis of the bisacetylene, 1,7-octadiyne, with trans-[Fe(dmpe)2(CH3)(C.tplbond.CPh)] (1a), was utilized to synthesize the bridged binuclear species trans,trans-[(CH3C.tplbond.C)Fe(dmpe)2[μ-C.tplbond.C(CH2)4C.tplbond.C]Fe(dmpe)2(C.tplbond.CO6H5)] (11). The trinuclear species trans,trans,trans-[(CO6H5C.tplbond.C)Fe(dmpe)2[μ-C.tplbond.C(CH2)4C.tplbond.C]Fe(dmpe)2[μ-C.tplbond.C(CH2)4C.tplbond.C]Fe(dmpe)2(C.tplbond.CO6H5)] (12) was synthesized by the photochem. reaction of Fe(dmpe)2(C.tplbond.CPh)(C.tplbond.C(CH2)4C.tplbond.CH) (6a) with Fe(dmpe)2(CH3)2. Extended irradiation of the bisacetylide complexes with phenylacetylene resulted in insertion of the terminal alkyne into one of the metal acetylide bonds to give acetylide butynene complexes. The structure of the acetylide butynene complex, trans-[Fe(dmpe)2(C.tplbond.CO6H4OCH3)[η-C(C6H5)CH(C.tplbond.CO6H4OCH3)]] (9a) was determined by single-crystal x-ray diffraction.
IT 425380-70-7P
RL: PPP (Properties); SW: (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)
RN 425380-70-7 CAPLUS
CN Iron, bis[1,2-ethanediylbis(dimethylphosphine)-K]][(4-

methoxyphenyl]ethynyl][[(1E)-4-(4-methoxyphenyl)-1-phenyl-1-buten-3-ynyl]-, (OC-6-11)- (3CI) (CA INDEX NAME)

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OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:673316 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 131:337589
TITLE: Electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene
AUTHOR(S): Fomina, Serguei; Fomina, Lioudmila; Gudasranna, Patricia
CORPORATE SOURCE: Universidad Nacional Autonoma Mexico, Inst de Investigaciones en Materiales, Coyocacan, 04510 CU, Mex.
SOURCE: THEOCHEM (1999), 488, 207-216
CODEN: THEODI; ISSN: 0166-1280
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Quantum-mech. calcs. of fully conjugated dendritic oligomers carried out at B3LYP/3-21G//HF/3-21G (d) and B3LYP/3-21G//PM3 levels of theory showed that loose dendritic architecture of β,β -dibromo-4-ethynyl styrene oligomers contributes little to the instability and conjugation disruption compared to 1 \rightarrow 2 branched polyacetylene, while Br terminal atoms in dendrimers strongly affect the electronic d. distribution in studied mols. On the one hand the bulky bromine atoms decrease the conjugation in Br-terminated dendrimers caused by steric hindrances, on the other hand, highly polarizable bromine atoms reduced significantly adiabatic ionization potentials (IPs) to be up to 1.5 eV lower than corresponding vertical potentials (IPv). Another phenomenon contributing to the reducing of IPs's of all dendrimers is the flattening of mol. geometry accompanying the ionization thus allowing better delocalization of pos. charge over the conjugated system while all aromatic ring except the very outer layer lost their aromaticity becoming essentially quinone by nature.

IT 206181-71-7 206181-72-8 206181-73-9
206181-74-0 206181-75-1 206181-75-2
206181-77-3 206181-78-4 206181-79-5

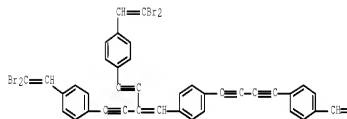
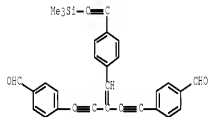
RI: PREP (Properties)
(electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene)

IT 425380-85-4
RI: SPW (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 425380-85-4 CAPLUS
CN Iron, [(1E)-1,4-bis(phenyl-1-buten-3-ynyl)bis[1,2-ethanediy]bis(dimethylphosphine-KP)] (phenylethynyl)-, (OC-6-11)- (3CI) (CA INDEX NAME)

RN 206181-71-7 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)

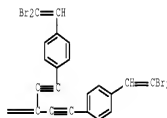
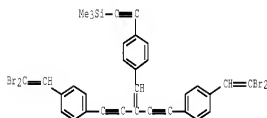
PAGE 1-A



RN 206181-72-8 CAPLUS

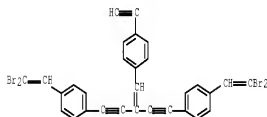
CN Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-

PAGE 1-B



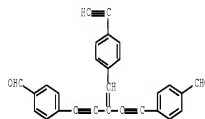
RN 206181-73-9 CAPLUS

CN Benzene, 1,1'-[3-[[4-(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)



RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



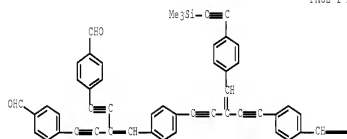
RN 206181-76-2 CAPLUS

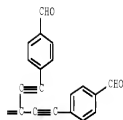
CN Benzaldehyde, 4,4'-[[3-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]]]bis- (9CI) (CA INDEX NAME)

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RN 206181-74-0 CAPLUS

CN Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

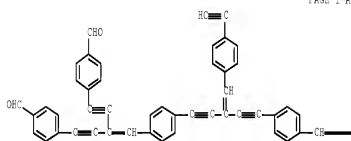
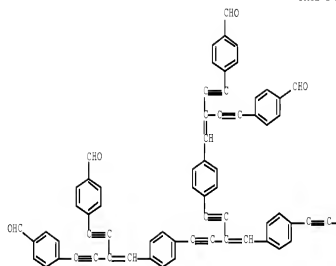




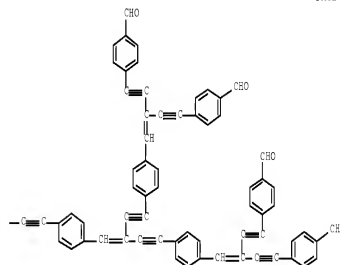
PAGE 1-B

RN 206181-77-3 CAPLUS

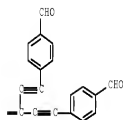
CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiene-1,5-diy]]bis[4,1-phenylene]3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



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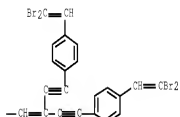
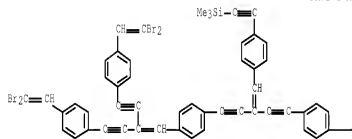


RN 206181-79-5 CAPLUS

CN Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]trimethyl- (9CI) (CA INDEX NAME)

RN 206181-78-4 CAPLUS

CN Benzaldehyde, 4,4'-[1,3-butadiene-1,4-diylbis(4,1-phenylene]3-[[4-[4-(4-formylphenyl)-2-[[4-(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene]3-[[4-(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

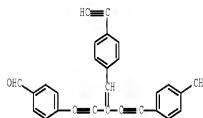


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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

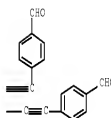
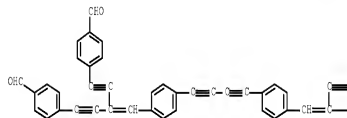
L4 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 1999:650836 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 132:16702
TITLE: Theoretical description of luminescent effects in
 β,β -di(4'-formylphenylethynyl)-4-ethynylstyrene
AUTHOR(S): Salcedo, R.; Guadarrama, P.; Sansores, L. E.; Fomine,
S.; Fomina, L.
CORPORATE SOURCE: Inst. de Investigaciones en Materiales, Inst. de
Investigaciones en Materiales, UNAM, Mexico, 04510,
Mex.
SOURCE: Materials Research Society Symposium Proceedings
(1999), 560 (Luminescent Materials), 359-364
CODEN: MRSPOH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Theor. calons. at HF/6-31 G(d) level were carried out on fully conjugated
comps. (4-ethynylbenzaldehyde, β,β -dikromo-4-ethynylstyrene, β,β -Di(4'-
formylphenylethynyl)-4-ethynylstyrene and its dimer) to understand the source
of blue emission observed in oligomers of the 1st and 2nd generation in CHCl₃
solns. The frontier orbitals are distributed through the framework of the
mols. (benzene rings, double and triple bonds and chromophores). Adnl., a CI
approach was applied over β,β -Di(4'-formylphenylethynyl)-4-ethynylstyrene

(compound 3) at CIS/6-31 G(d) level to modeling excited states and simulate
the UV-visible spectrum exptl. obtained. Calculated transitions corresponded
to 50-51 which are, presumably, responsible for the fluorescence observed
20181-75-1 251479-84-2
R1: PEP (Physical, engineering or chemical process); PRP (Properties);
PSC (Process)
(theor. description of luminescent effects in styrene derivs.)
RN 206162-75-1 CAPLUS
CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-
diyl]bis- (CA INDEX NAME)



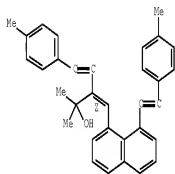
RN 251479-84-2 CAPLUS
CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis(4,1-phenylene[3-[(4-
formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1998:269262 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 128:257221
 ORIGINAL REFERENCE NO.: 128:50919a,50922a
 TITLE: Steric Hindrance Facilitated Synthesis of Enynes and Their Intramolecular [4 + 2] Cycloaddition with Alkynes
 AUTHOR(S): Gonzalez, Juan J.; Francesch, Andres; Cardenas, Diego J.; Echavarren, Antonio M.
 CORPORATE SOURCE: Departamento de Química Orgánica, Universidad Autónoma de Madrid, Madrid, 28049, Spain
 SOURCE: Journal of Organic Chemistry (1998), 63(9), 2854-2857
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 128:257221
 AB The palladium-catalyzed insertion of 1-alkynes into internal alkynes which are bent out of linearity by the interference with a peri or ortho substituent led to enynes regioselectively. The resulting enynes undergo a new type of intramolecular thermal cycloaddition, which can be used for the annulation of an aryl ring onto naphthalene derivatives to afford fluoranthenes. The cyclization of [E]-1-(1-buten-3-ynyl)-8-ethynynaphthalene could also be performed in the presence of a Cu(I) catalyst at room temperature
 IT 205121-59-44
 RI: SPW (Synthetic preparation); PREP (Preparation) (preparation of enynes and their intramolecular [4+2]cycloaddition with alkynes)
 RN 205124-39-6 CAPLUS
 CN 4-Pentyn-2-ol, 2-methyl-5-(4-methylphenyl)-3-[(8-(2-(4-methylphenyl)ethynyl)-1-naphthalenyl)methylene]-, (3Z)- (CA INDEX NAME)

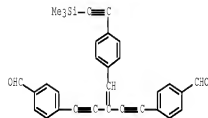
Double bond geometry as shown.



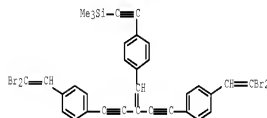
OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)
 REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1998:247633 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 128:295129
 ORIGINAL REFERENCE NO.: 128:58501a,58504a
 TITLE: Synthesis and characterization of well-defined fully conjugated hyperbranched oligomers of β,β -dibromo-4-ethynylstyrene

AUTHOR(S): Fomina, Lioudmila; Guadarrama, Patricia; Fomina, Serquel; Salcedo, Roberto; Ogawa, Takeshi
 CORPORATE SOURCE: Instituto Investigaciones Materiales, Univ. Nacional Autónoma de México, México, 04510, Mex.
 SOURCE: Polymer (1998), 39(12), 2629-2635
 CODEN: POLMAG; ISSN: 0032-3861
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Well-defined dendritic oligomers of poly(β,β -dibromo-4-ethynylstyrene) of the first and second generation were synthesized by a stepwise synthesis, and characterized. NMR and theoretical calculations showed that free rotation around formal single bonds is hampered by conjugation. All of the oligomers were blue emitters with their emission maxima correlating with the number of repeating units. All dendrimers except β,β -bis[β' -di(β'' -dibromostyryl)-4'-ethynyl]styryl-4'-ethynyl-4-ethynylstyrene showed two maxima in the excitation spectra.
 IT 206181-71-70 206161-72-66 206181-73-39
 206181-74-66 206181-75-1F 206181-76-2P
 206181-77-3V 206181-78-4P
 RI: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RMC (Reactant or reagent) (preparation and characterization of conjugated hyperbranched β,β -dibromo-4-ethynylstyrene oligomers)
 RN 206181-71-70 CAPLUS
 CN Benzaldehyde, 4,4'-[3-[[4-[[4-trimethylsilyl]ethynyl]phenyl]methylene]-1,4-pentadiene-1,5-diyl]bis- (9CI) (CA INDEX NAME)

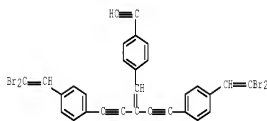


RN 206181-72-8 CAPLUS
 CN Silane, [[4-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



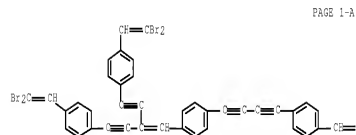
RN 206181-73-9 CAPLUS

CN Benzene, 1,1'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)

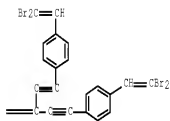


RN 206181-74-0 CAPLUS

CN Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-(2,2-dibromomethenyl)phenyl]-2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



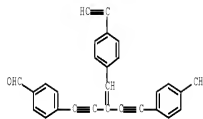
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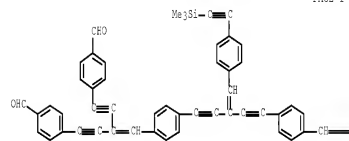
RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

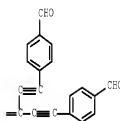


RN 206181-76-2 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-[(trimethylsilyl)ethynyl]phenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



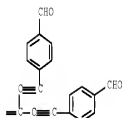
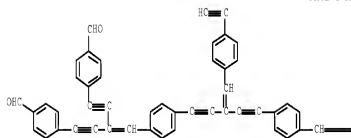
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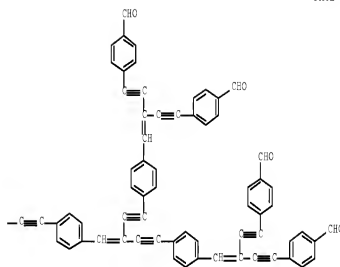
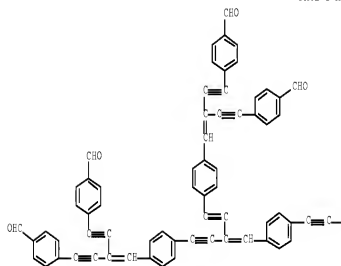
RN 206181-77-3 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 206181-78-4 CAPLUS

CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis(4,1-phenylene[3-[[4-(4-(4-formylphenyl)-2-[[4-(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yn-4,1-diyl]-4,1-phenylene[3-[[4-(4-formylphenyl)ethynyl]-3-buten-1-yn-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

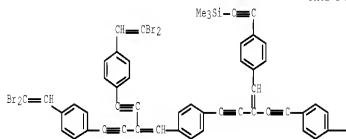


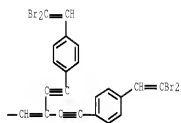
IT 206181-78-5P

RI: FRP (Properties); SFM (Synthetic preparation); PREP (Preparation)
(preparation and characterization of conjugated hyperbranched
β,β-dibromo-4-ethynylstyrene oligomers)

RN 206181-79-5 CAPLUS

CN Silane, [[4-(4-(4-(4-(2,2-dibromoethenyl)phenyl)-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl)-2-[[4-(4-(2,2-dibromoethenyl)phenyl)-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 1996:303100 CAPLUS Full-text

DOCUMENT NUMBER: 125:11582

ORIGINAL REFERENCE NO.: 125:2539a,2542a

TITLE: Synthesis and polymerization of

β,β -dibromo-4-ethynylstyrene; preparation of

a new polyconjugated, hyperbranched polymer

AUTHOR(S): Fomina, Lioudmila; Salcedo, Roberto

CORPORATE SOURCE: Inst. Investigaciones Materiales, Circuito Exterior,

Ciudad Univ., Mexico City, 04510, Mex.

SOURCE: Polymer (1996), 37(9), 1723-1728

CODEN: POLMAG; ISSN: 0032-3661

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

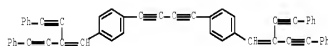
AB The monomer, β,β -dibromo-4-ethynylstyrene, was prepared and polymerized by the Heck reaction to give a partially soluble, conjugated hyperbranched polymer. The polymer structure was elucidated using standard spectroscopic techniques and with the aid of model compound synthesis. Theor. calcons. using the AM1 method were carried out and showed that conjugation in the polymer is partially disrupted by twisting of the benzene rings. Both the model compound and the polymer showed luminescence.

IT 177426-40-1P

RI: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (model compound for dihomomethylstyrene polymer)

RN 177410-40-1 CAPLUS

CN Benzene, 1,1'-[1,3-butadiene-1,4-diyl]bis[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]-] (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L4 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 1995:946580 CAPLUS Full-text

DOCUMENT NUMBER: 124:9540

ORIGINAL REFERENCE NO.: 124:2031a,2034a

TITLE: Novel polymers containing discrete conjugated units, produced by the Heck reaction

AUTHOR(S): Fomina, Sergel; Fomina, Lioudmila; Florentino, Hector

Quiroz; Mander, Juan Manuel; Ogawa, Takeshi

CORPORATE SOURCE: Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Coyoacan, 04510, Mex.

SOURCE: Polymer Journal (Tokyo) (1995), 27(11), 1085-93

CODEN: POLJBJ; ISSN: 0032-3896

PUBLISHER: Society of Polymer Science, Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Novel monomers and polymers containing arylenevinylideneethynylene groups were synthesized via the Heck reaction. The polymers were amorphous and soluble in common organic solvents. They have T_g approx. 60°, 5% weight loss at 240-340° and undergo thermal crosslinking at 170-190° with loss of triple bonds. One of the polymers exhibits strong blue luminescence with emission maxima approx. 380-390 and 470-480 nm with excitation at 320 nm. All polymers show 3rd order MLO susceptibility approx. 10-10 esu.

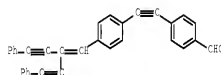
IT 171296-95-0P

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; in preparation of polyacetylene-polyesters)

RN 171296-95-0 CAPLUS

CN Benzaldehyde, 4-[2-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]ethynyl]- (CA INDEX NAME)



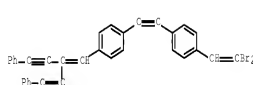
IT 171296-95-0P

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(monomer; in preparation of polyacetylene-polyesters)

RN 171296-95-1 CAPLUS

CN Benzene, 1-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



IT 171296-99-4P

RL: FRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, characterization and properties of)

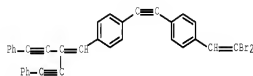
RN 171296-99-4 CAPLUS

CN Decanedioic acid, di-2-propynyl ester, polymer with 1-[[4-(2,2-dihydroxyethyl)phenyl]ethynyl]-4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]benzene (RCT) (CA INDEX NAME)

CM 1

CRN 171296-96-1

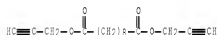
CMF C34 H20 Br2



CM 2

CRN 93164-22-8

CMF C16 H22 O4



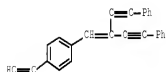
IT 171297-01-2, β,β -Bis(phenylethynyl)-4-ethynylstyrene

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; in preparation of polyacetylene-polystyrenes)

RN 171297-02-2 CAPLUS

CN Benzene, 1-ethynyl-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L4 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:642218 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 123:33763

ORIGINAL REFERENCE NO.: 123:6259a,6262a

TITLE: Synthesis and molten-state polymerization of some novel conjugated diacetylenes

AUTHOR(S): Fomina, Lioudmila; Allier, Hector; Fomina, Sergel; Salcedo, Roberto; Ogawa, Takeshi

CORPORATE SOURCE: Inst. Investigaciones Materiales, Ciudad Univ., Mexico, 04510, Mex.

SOURCE: Polymer Journal (Tokyo) (1995), 27(6), 591-600
CODEN: POLJDB; ISSN: 0032-3996

PUBLISHER: Society of Polymer Science, Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of new, highly conjugated diacetylenes, 4-ethynylstilbene derivs., was synthesized and their polymerization was studied. None of them was found to undergo topochem. polymerization in the solid state but they readily polymerized in the molten state to give red transparent and amorphous polymers. All the polymers had an absorption maximum in the visible spectra around 500 nm, and FT-IR data showed the enyne structure of the polymer chain resulted from 1,4-addition

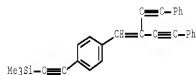
IT 164467-50-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of ethynylstilbene derivative monomers)

RN 164467-30-5 CAPLUS

CN Benzene, 1-[[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-4-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



IT 164467-25-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and characterization of polydiacetylenes from ethynylstilbene derivs. in molten state)

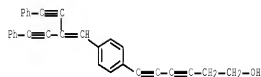
RN 164467-25-8 CAPLUS

CN 3,5-Hexadiyn-1-ol, 6-[[4-(4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]phenyl]-, homopolymer (RCT) (CA INDEX NAME)

CM 1

CRN 164467-20-3

CMF C30 H20 O

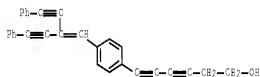


IT 164467-20-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and polymerization of)

RN 164467-20-3 CAPLUS

CN 3,5-Bisazidyn-1-ol, 6-(4-(4-phenyl-2-(2-phenylethynyl)-1-butan-3-yn-1-yl)phenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
RECORD (11 CITINGS)

L4 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1994:522234 CAPLUS Full-text

DOCUMENT NUMBER: 121:122234

ORIGINAL REFERENCE NO.: 121:21823h,21826a

TITLE: Difluoride derivative and liquid crystal composition
containing the same

INVENTOR(S): Yokokoji, Osamu; Irisawa, Jun; Koh, Hidemasa

PATENT ASSIGNER(S): Asahi Glass Co., Ltd., Japan

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIKX02

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

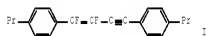
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405613	A1	1994/0317	WO 1993-JP1235	1993/0901
R: US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 628528	A1	1994/1214	EP 1993-9196/2	1993/0901
R: DE, FR, GB, IT				
JP 06263661	A	1994/0920	JP 1993-219709	1993/0903
JP 3564711	B2	2004/0915		
US 5419851	A	1995/0530	US 1994-211625	1994/0420
JP 2004292454	A	2004/1021	JP 2004-115211	2004/0409
JP 3707493	B2	2005/1019		
PRIORITY APPLN. INFO.:				
			JP 1992-263027	A 1992/0904
			WO 1993-JP1235	W 1993/0901
			JP 1993-219709	A3 1993/0903

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LISTS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:122234

GI



AB Difluoride derivs. represented by the general formula:

R1(R1Y1)m2Q(CFC.tgpbond.CA3(Y2A1)nR2 (A1 - A4 = trans-1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene wherein Σ CH groups of each ring may be substituted by 0 or Σ CH2 groups of the ring may be substituted by 0 or S; m, n = 0, 1; R1, R2 = C1-10 alkyl, halo, cyano wherein (1) C, CO2, or C2C may be inserted between the C-C bond of alkyl or that between alkyl and ring, (2) a part of the C-C bonds in alkyl is replaced by C=C or C.tgpbond.C bond, or (3) one CH2 group in alkyl is replaced by CO group; Y1, Y2 = CO2, C2C, C.tgpbond.C, CH2CH2, CH=CH, OCH2, CH2O) are prepared These compds. have low viscosity, are light-stable, and hence can provide a liquid crystal composition having high response speed. Thus, 0.1 mol ClCF3CF2 was blown into THF at -100° followed by adding dropwise 62.1 mL 1.61 M BuLi/hexane, stirring for 30 min, adding dropwise 0.1 mol Me3SiCl, stirring for 1 h, adding dropwise a solution of 4-propylphenyl lithium in THF (prepared from 4-propylidobenzene and BuLi) at -100°, and stirring for 2 h at 0° to give 75% (Z)-4'-PrC6H4CF3CF2. The latter compound (0.075 mol) was reacted with 0.15 mol HF in aqueous MeCN at 70° for 1 h to give 63% (E)-4'-PrC6H4CF3CF2 which (0.062 mol) was dissolved in THF, cooled to -78°, and treated dropwise with 38.5 mL 1.61 M BuLi/hexane followed by stirring for 30 min, adding 15.7 g iodine, and stirring at room temperature for 2 h to give 63% (E)-4'-PrC6H4CF3CF2. The latter compound (0.051 mol) and 0.051 mol 4-propylphenylacetylene were dissolved in 100 mL Et3N followed by adding Pd(PPh3)2Cl2 and CuI and the resulting mixture was allowed to react at room temperature for 6 h to give 70% diphenyldifluorobutene derivative (I). A STM-type liquid crystal display device was prepared from a liquid composition containing 20 weight% I and 80 weight% ZLI-1565 and irradiated with a UV carbon arc lamp for 200 h; new compds. were hardly formed whereas cis-4,4'-bis(n-propyl)difluorostilbene was formed in a liquid crystal composition containing ZLI-1565 and trans-4,4'-bis(n-propyl)difluorostilbene.

IT 156869-08-8P

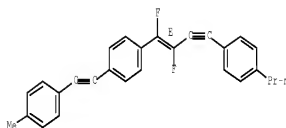
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as liquid crystal with UV stability and low viscosity)

RN 156869-08-8 CAPLUS

CN Benzene, 1-[(1,2-difluoro-4-(4-propylphenyl)-1-butan-3-ynyl]-4-[(4-methylphenyl)ethynyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



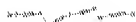
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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chain nodes :
2 3 4 5 6 7 8 9 10 11 12 13 14 15 20 24
chain bonds :
2-3 2-24 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15
15-20
exact/norm bonds :
2-3 2-24 8-9 9-10 15-20
exact bonds :
3-4 4-5 5-6 6-7 7-8 10-11 11-12 12-13 13-14 14-15

G1:Cb,Cy,By

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,By

Match level :
2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 20:CLASS 24:CLASS

L5 STRUCTURE UPLOADED

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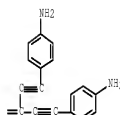
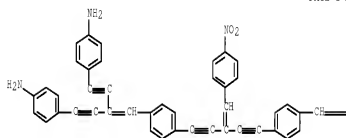
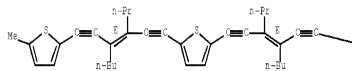
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L7 32 L6

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L7 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2009:1099083 CAPLUS Full-text
DOCUMENT NUMBER: 151:508432
TITLE: Hybrid Conjugated Organic Oligomers Consisting of Oligodiacetylene and Thiophene Units: Synthesis and Optical Properties
AUTHOR(S): Pliak, Gregor S.; van Grujthuljeen, Kitty; van Doorn, Reindert H.; van Lagen, Barend; Suijhoelter, Ernst J. R.; Zuilhof, Han
CORPORATE SOURCE: Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, Wageningen, 6703 HB, Neth. Chemistry--A European Journal (2009), 15(36), 9085-9096, S9085/1-S9085/19
SOURCE: CODEN: CHEMUD; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 151:508432
AB Novel and highly soluble hybrid conjugated organic oligomers consisting of oligodiacetylene and thiophene units have been synthesized in high purity through iterative and divergent approaches based on a sequence of Sonogashira reactions. The series of thiophene-containing oligodiacetylenes and homocoupled oligodiacetylenes show, both in solution and in the solid state, a strong optical absorption, which is progressively red shifted with increasing chain length. The linear correlation of the absorption maximum with the inverse of conjugation length (CL = number of double and triple bonds) shows that the effective conjugation length of this system is extended up to at least CL = 20. Furthermore, absorption measurements of dropcast thin films display not only a bathochromic shift of the absorption maxima but also a higher wavelength absorption, which is attributed to increased π - π interactions. The wavelength of the maximum fluorescence emission also increases with CL, and emission is maximal for oligomers with CL = 7-12 (fluorescence quantum yield Φ_F = .apprx.0.2). Both longer and shorter oligomers display marginal emission. The calculated Stokes shifts of these planar materials are relatively large (0.4 eV) for all oligomers, and likely due to excitation to the S2 state, thus suggesting that the presence of enyne moieties dominates the ordering of the lowest excited states. The fluorescence lifetimes (τ_F) are short (τ_{Fmax} = <1 ns) and closely follow the tendency obtained for the fluorescence quantum yield. The anisotropy lifetimes show a near-linear increase with CL in line with highly rigid oligomers.
IT 1192820-79-3P
R1: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis via iterative Sonogashira coupling and optical properties of hybrid conjugated organic oligomers consisting of oligodiacetylene and thiophene units)
RN 1192820-79-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED
Double bond geometry as shown.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2009:76616 CAPLUS Full-text

DOCUMENT NUMBER: 150:167710

TITLE: Push-pull hyperbranched molecules. A theoretical study

AUTHOR(S): Ramos, Estrella; Guadarrama, Patricia; Teran, Gerardo;

Fomine, Serguei

CORPORATE SOURCE: Instituto de Investigaciones en Materiales,
Universidad Nacional Autonoma de Mexico, Mexico,
04510, Mex.

SOURCE: Journal of Physical Organic Chemistry (2009), 22(1),
9-16

CODEN: JPOCHE; ISSN: 0894-3230

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electronic properties of the ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups have been studied at BEIR/cc-pvdz//HF/6-31g(d), TD-BEIR/cc-pvdz//HF/6-31g(d) and TD-BEIR/cc-pvdz//CIS/6-31g(d) levels of theory, resp. It was demonstrated that dendritic architecture of push-pull mols. favors the charge transfer in the excited state compared to linear mols. The possibility of adopting a plane conformation is an important condition for the charge transfer in an excited state. According to the calcs. 1:1 ratio of donor and acceptor groups is another important precondition for the manifestation of strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the $S_0 \rightarrow S_1$ transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

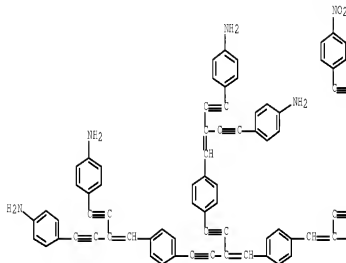
IT 1107616-71-6 1107616-72-7 1107616-73-8

RI: FRP (Properties)

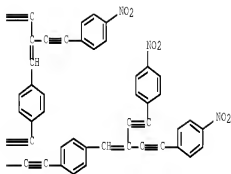
(electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

RN 1107616-71-6 CAPLUS

CN Benzenamine, 4,4'-[3-[[[4-[5-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-nitrophenyl]methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyn-1-yl]bis-

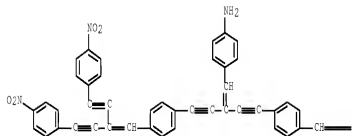


PAGE 1-B

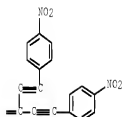


RN 1107616-73-8 CAPLUS
 CN Benzenamine, 4-[4-[4-(4-(4-nitrophenyl)-2-(2-(4-nitrophenyl)ethynyl)-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-(4-nitrophenyl)-2-(2-(4-nitrophenyl)ethynyl)-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT 1107616-76-1

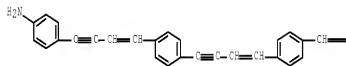
RL: PPP (Properties)

(linear analog; electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

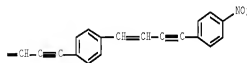
RN 1107616-76-1 CAPLUS

CN Benzenamine, 4-[4-[4-(4-(4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl)-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2008:355050 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:520471

TITLE: Tetrafulerene Conjugates for All-Organic Photovoltaics

AUTHOR(S): Fernandez, Gustavo; Sanchez, Luis; Veldman, Dirk; Wienk, Martijn M.; Atienza, Carmen; Galdi, Dirk M.; Janssen, Rene A. J.; Martin, Nazario

CORPORATE SOURCE: Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Madrid, 28040, Spain

SOURCE: Journal of Organic Chemistry (2008), 73(8), 3189-3196 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:520471

AB The synthesis of two new tetrafulerene nanoconjugates in which four C60 units are covalently connected through different π -conjugated oligomers (oligo(p-phenylene ethynylene) and oligo(p-phenylene vinylene)) is described. The photovoltaic response of these C60-based conjugates was evaluated by using them as the only active material in organic solar cells, showing a low photovoltaic performance. Photophys. studies in solution demonstrated a very fast (.apprx.10 ps) deactivation of the singlet excited state of the central core unit to produce both charge-separated species (i.e., C60^{•-}-oligomer^{•+}

(C60)3 and C60 centered singlet excited states). The charge-separated state recombines partly to the C60 centered singlet state that undergoes subsequent intersystem crossing. Photophys. studies carried out in films support these data, exhibiting long-lived triplet excited states. For both tetraphenylene arrays, the low yield of long-lived charge carriers in thin films accounts for the limited photovoltaic response. On the contrary, utilizing the oligo(p-phenylene vinylene) centered precursor aldehyde as an electron donor and antennae unit and mixing with the well-known C60 derivative PCBM, the photophys. studies in films show the formation of long-lived charges. The photovoltaic devices constructed from these mixts. showed a relatively high photocurrent of 2 mA/cm2. The sharp contrast between the nanoconjugates and the phys. blends tentatively was attributed to improved charge dissociation and the collection of more favorable energy levels in the blends as a result of partial aggregation of both of the components.

IT 1022991-37-29

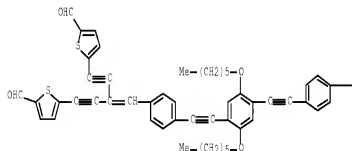
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(In synthesis of tetraphenylene conjugates for all-organic photovoltaics)

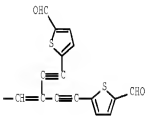
RN 1022991-37-2 CAPLUS

CN 2-Thiophenecarboxaldehyde, 5,5'-[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-[2-(5-formyl-2-thienyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 CF 32 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2008:244421 CAPLUS Full-text

DOCUMENT NUMBER: 148:403337

TITLE: Triphenylphosphine Incorporation Reactions of Diynyl Complexes containing a Tpru(NO) Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene
Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Renta; Umakoshi, Keisuke; Onishi, Masayoshi

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan

SOURCE: Organometallics (2008), 27(6), 1227-1233

CODEN: ORGM7D; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:403337

AB Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand (Tp = B[pyrazol-1-yl]3) were prepared, and their reactivities toward PPh3 incorporation in the presence of HBF4·Et2O were described. The PPh3 incorporation of mono(arylbutadiynyl) complex TpRuCl(C.tpbond.C-C.tpbond.C-C6H4Me)(NO) (1) resulted in the β-phosphinoalkenyl complex [E]-[TpRuCl(CH3C(PPh3)-C.tpbond.C-C6H4Me)(NO)]BF4 (2-BF4), whereas when bis(arylbutadiynyl) TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)2(NO) (3) was treated, mono- and bis β-phosphinoalkenyl complexes [E]-[TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)(CH3C(PPh3)-C.tpbond.C-C6H4Me)(NO)]BF4 (4-BF4) and [E,E]-[TpRu(CH3C(PPh3)-C.tpbond.C-C6H4Me)2(NO)]BF4 (5-BF4) were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutadiynyl) (3-hydroxyalkenyl) complex, TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)(C.tpbond.CCPH2(OH))(NO) (6), was allowed to react with PPh3 in the presence of the protic acid to give the α-phosphinoalkenyl [TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)(C(PPh3):C:CPH2(NO)]BF4 (7-BF4). Interestingly, thermal isomerization of 7-BF4 to a ruthena-2-PPh3-cyclobuta[b]naphthalene [TpRu(CH(PPh3)[3-Ph-8-(MeC6H4-C.tpbond.C-C)ClO4]](NO)]BF4 (8-BF4) was observed

IT 1015477-27-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(triphenylphosphine incorporation reactions of diynyl complexes containing pyrazolylboratoruthenium nitrosyl fragment and isomerization to ruthenacyclobutanaphthalene)

RN 1015477-27-6 CAPLUS

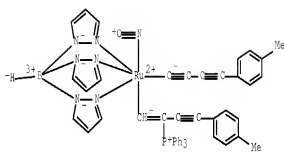
CN Ruthenium[1+], [hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2'] [4-(4-methylphenyl)-1,3-butadiyn-1-yl] [(1E)-4-(4-methylphenyl)-2-(triphenylphosphonio)-1-buten-3-yn-1-yl]nitrosyl-, (OC-6-24)-, tetrafluoroborate[1-] (1:1) (CA INDEX NAME)

CM 1

CN 1015477-26-5

CM C49 H40 B N7 O P Ru

CCI CCS



CM 2

CRN 14874-70-5
CME B F4
CCI CCS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN
ACCESSION NUMBER: 2007:1105260 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 148:11306
TITLE: Formation and Structural and Dynamic Features of
Atropisomeric η^2 -Iminoacyl Zirconium Complexes
AUTHOR(S): Spies, Patrick; Kehr, Gerald; Mehr, Seda; Froehlich,
Roland; Erier, Gerhard
CORPORATE SOURCE: Organisch-Chemisches Institut, Universitaet Muenster,
Muenster, 48149, Germany
SOURCE: Organometallics (2007), 26(23), 5612-5620
CODEN: ORGMD7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
SOURCE(S): CASREACT 148:11306
AB The $\text{Cp}_2\text{ZrCl}(\text{CPh}(\text{C}(\text{PX})_2\text{C}(\text{tpbond}.\text{CPh}))$ complexes 7a (X = Ph) and 10 (X = C6F5)
insert tert-butylisocyanide into the $\text{Zr}-\text{C}(\text{sp}^2)-\text{C}$ bond to yield the iminoacyl
zirconocene complexes, $\text{Cp}_2\text{ZrCl}(\text{C}(\text{HCMe}_3)\text{CPh}(\text{C}(\text{PX})_2\text{C}(\text{tpbond}.\text{CPh}))$ 13a and 13b.
X-ray crystal structure anal. of complexes 13a and 13b revealed a chiral
atropisomeric structure with a torsion angle of $74.8(2)^\circ$ (13a) and $72.9(6)^\circ$
(13b), resp., around the central iminoacyl/alkenyl $\text{C}(\text{sp}^2)-\text{C}(\text{sp}^2)-\text{C}$ bond. In
solution an analogous chiral structure is observed. The barrier of
interconversion of the enantiomeric atropisomers of 13a and 13b was determined
at $\Delta G_{\text{thermod.}}$ (327K) = 14.9 ± 0.3 kcal mol $^{-1}$ (13a) and $\Delta G_{\text{thermod.}}$ (325K) =

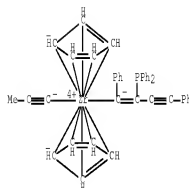
14.8 ± 0.3 kcal mol $^{-1}$ (13b) by temperature-dependent dynamic NMR spectroscopy.
Reaction of 7a and 10 with methylolithium followed by treatment with $\text{B}(\text{C}_6\text{F}_5)_3$
gave the corresponding cationic zirconocene complexes
 $\text{Cp}_2\text{Zr}^+(\text{THF})(\text{CPh}(\text{C}(\text{PX})_2\text{C}(\text{tpbond}.\text{CPh}))[\text{MeB}(\text{C}_6\text{F}_5)_3]$ 12a and 12b. These
complexes took up 2 mol equiv of tert-butylisocyanide to yield the cationic N-
inside η^2 -iminoacyl zirconocene systems 14a and 14b as isonitrile adducts.
The cationic complexes 14a and 14b are also axially chiral. The barriers of
enantiomerization ($\Delta G_{\text{thermod.}}$ (288 K) = 13.1 ± 0.3 kcal mol $^{-1}$ (14a),
 $\Delta G_{\text{thermod.}}$ (293 K) = 13.4 ± 0.3 kcal mol $^{-1}$ (14b)) were also determined by
dynamic NMR spectroscopy.

IT 956475-66-04P

RI: PRP (Properties); SPW (Synthetic preparation); PREP (Preparation)
(crystal structure; isonitrile insertion reaction into neutral and
cationic butenylzirconocene complexes to give atropisomeric iminoacyl
zirconocene complexes)

RN 958635-66-0 CAPLUS

CN Zirconium, bis(η^5 -2,4-cyclopentadien-1-yl)(1E)-2-(diphenylphosphino)-
1,4-diphenyl-1-butan-3-yn-1-yl-1-propyn-1-yl- (CA INDEX NAME)



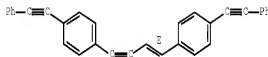
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN
ACCESSION NUMBER: 2007:995140 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 147:448227
TITLE: Convenient synthesis of (1-propynyl)arenes through a
one-pot double elimination reaction, and their
conversion to arynes
AUTHOR(S): An, De-Lie; Zhang, Zhiyang; Orita, Akihiro; Mineyama,
Hidetaka; Otera, Junzo
CORPORATE SOURCE: Department of Chemistry, College of Chemistry and
Chemical Engineering, Hunan University, Changsha,
410082, Peop. Rep. China
SOURCE: Synlett (2007), (12), 1909-1912
CODEN: SYNLDE; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:448227
AB A series of prop-1-ynyl arenes were prepared by one-pot double elimination
reaction of EtSO $_2$ Ph, aromatic aldehyde, and $\text{CIP}(\text{OEt})_2$ in THF with a base such

as BuLi and t-BuOK. A propargyllithium, which was prepared by treatment of propyn-1-yl arene with BuLi in the presence of 1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMFO), reacted with aromatic aldehyde, ClPO(OEt)₂ and t-BuOK to afford 4-arylbut-3-en-1-ynyl arene. Photoluminescence of the enynes thus prepared was recorded both in solution and in the solid state.

IT 951766-78-2P
 RL: SPW (Synthetic preparation); PREP (Preparation)
 (preparation of propargyl arenes through one-pot double elimination and conversion to enynes)
 RN 951766-78-2 CAPLUS
 CN Benzene, 1,1'-(1E)-1-buten-3-ynyl-4,4'-diylbis[4-(2-phenylethynyl)]- (CA INDEX NAME)

Double bond geometry as shown.



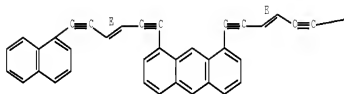
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STM
 ACCESSION NUMBER: 2007:46877 CAPLUS Full-text
 DOCUMENT NUMBER: 148:284829
 TITLE: Synthesis of smallest unit model of graphite intercalation compound and its possibility
 AUTHOR(S): Ogoshi, Senuke
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Osaka University, Japan
 SOURCE: Asahi Gassu Zaidan Jishi Kenkyu Seika Hokoku (2006) 01.03.07/01.03.07/8
 CODEN: AGSHEN; ISSN: 0919-9179
 PUBLISHER: Asahi Gassu Zaidan
 DOCUMENT TYPE: Journal; (computer optical disk)
 LANGUAGE: Japanese
 OTHER SOURCE(S): CASREACT 148:284829
 AB Graphite is perhaps the simplest layered structure. Many substances can be intercalated between layers of graphite. Upon intercalation, the graphite layers moved apart somewhat due to the intercalated atom. However, the layers still keep parallel each other which would be the key for the formation of intercalation compds. Thus, compds. having two aromatic rings, which can change the distance between the rings and keep parallel to each other, were designed and synthesized. The target compound was 1,8-bis[6-(1-naphthalenyl)-3-hexene-1,5-diynyl]anthracene.

IT 1007602-95-0P
 RL: SPW (Synthetic preparation); PREP (Preparation)
 (preparation of bis[1(naphthalenyl)hexenediynyl]anthracene (smallest unit model for graphite intercalation compound))
 RN 1007602-95-0 CAPLUS
 CN Anthracene, 1,8-bis[3E)-6-(1-naphthalenyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



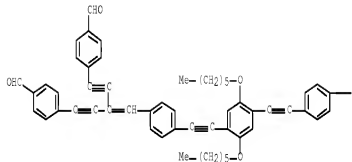
L7 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STM
 ACCESSION NUMBER: 2006:82014 CAPLUS Full-text
 DOCUMENT NUMBER: 144:334153
 TITLE: Light harvesting tetrafullerene nanoarray for organic solar cells
 AUTHOR(S): Atienza, Carmen M.; Fernandez, Gustavo; Sanchez, Luis; Martin, Nazario; Dantas, Ines Sa; Wienk, Martijn M.; Janssen, Rene A. J.; Rahman, G. M. Amir; Guldi, Dirk M.
 CORPORATE SOURCE: Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense, Madrid, E-28040, Spain
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (5), 514-516
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:334153

AB A light absorbing π -conjugated oligomer-tetrafullerene nanoarray was synthesized and its photophys. study reveals an intramol. energy transfer. A photovoltaic device fabricated from this nanoarray and poly[3-hexylthiophene] shows an external quantum efficiency of 15% at 500 nm.

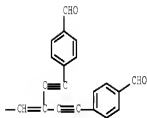
IT 880486-74-8P
 RL: PREP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PYP (Physical process); RCT (Reactant); SPW (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (compound 4; light harvesting tetrafullerene nanoarray for organic solar cells)
 RN 880486-74-8 CAPLUS
 CN Benzaldehyde, 4,4'-[[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl]-4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-ynyl-4,1-diyl]]bis-

(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 20051004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNER(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005086176	A1	20050915	NO 2005-JP3950	20050309
W:	AE, AG, AL, AM, AT, AU, A2, BA, BB, BG, BR, BW, BY, BZ, CA, CH,			

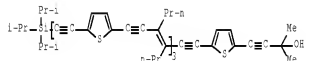
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, ST, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZH
BN: BM, GE, GM, KE, LS, MW, MZ, NA, SD, SI, SZ, TG, UG, ZM, ZW, AG, AI, AY, BG, BZ, KE, MD, RU, UZ, UY, VE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MJ, NL, PL, PT, RO, SE, SI, SK, TR, BE, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NG, SN, TD, TG

US 20070176164 A1 20070802 US 2007-591350 20070307
PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309
WO 2005-JP3950 W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title comps. are useful as electroluminescent devices.

IT 740810-64-4P 744315-65-5P 740810-67-7P
740810-68-6P 866533-36-5P 866831-87-6P
866594-01-5P 866884-02-6P 866884-11-7P
866594-12-8P 866884-13-8P 866594-15-3P
866884-19-4P 866884-19-4P 866594-31-4P
866884-32-2P

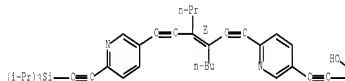
RU: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

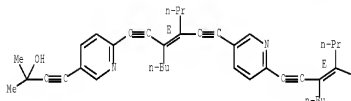


RN 740810-65-5 CAPLUS

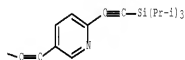
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

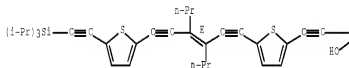


RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

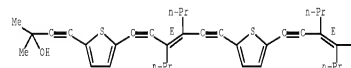


RN 740810-68-8 CAPLUS

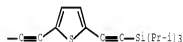
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



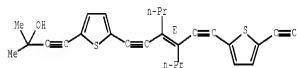
PAGE 1-B



RN 864683-96-5 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

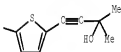
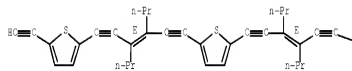
Double bond geometry as shown.



RN 864683-97-6 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

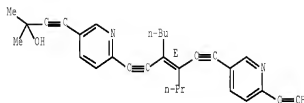
Double bond geometry as shown.



RN 864684-01-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

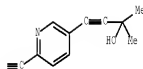
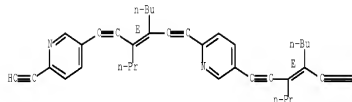
Double bond geometry as shown.



RN 864684-02-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

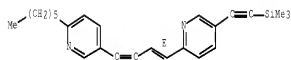
Double bond geometry as shown.



RN 864684-11-7 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

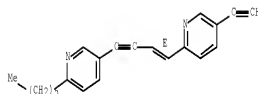
Double bond geometry as shown.



RN 864684-12-8 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

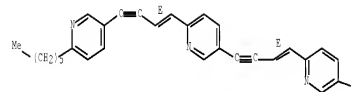
Double bond geometry as shown.



RN 864684-13-9 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[(3E)-4-[5-[2-(trimethylsilyl)ethynyl]-2-pyridinyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



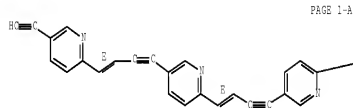
PAGE 1-B



RN 864684-15-1 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-butan-3-yn-1-yl]-3-pyridinyl)-1-butan-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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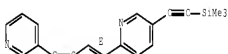
PAGE 1-B



RN 864684-18-4 CAPLUS

CN Pyridine, 2-[(1E)-4-(3-pyridinyl)-1-butan-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

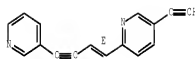
Double bond geometry as shown.



RN 864684-19-5 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(3-pyridinyl)-1-butan-3-yn-1-yl]- (CA INDEX NAME)

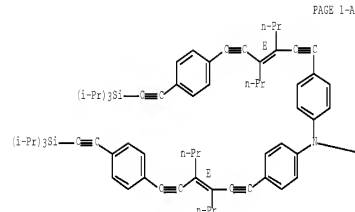
Double bond geometry as shown.



RN 864684-31-1 CAPLUS

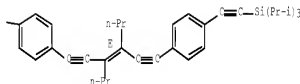
CN Benzanamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-(4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl)ethynyl]-3-heptan-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-(4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl)ethynyl]-3-heptan-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



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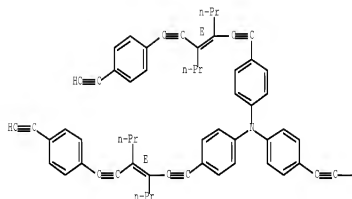
RN 864684-32-2 CAPLUS

CN Benzanamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-

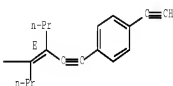
penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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IT 740810-66-6P 740810-69-3P 864684-03-7P
 864684-05-7P 864684-03-3P 864684-15-2P
 864684-17-3P 864684-10-8P 864684-21-5P
 864684-22-7P 864684-23-1P 864684-24-1P
 864684-25-7P 864684-26-4P 864684-27-5P
 864684-28-4P 864684-23-7P 864684-30-0P
 864684-33-3P

RU: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic

electroluminescent devices)

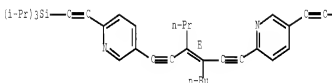
RN 740810-66-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-

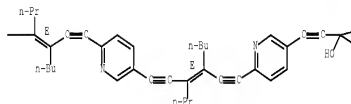
butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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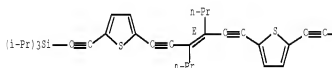


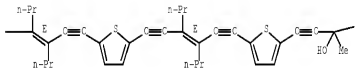
RN 740810-69-9 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

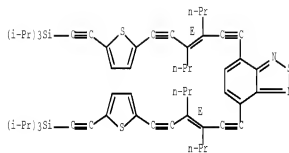
Double bond geometry as shown.

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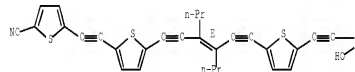
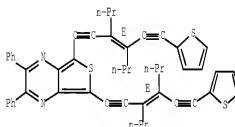
PAGE 1-C

RN 864684-09-3 CAPLUS
CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyne-1-yl]-2,3-diphenyl-1-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 864684-03-7 CAPLUS
CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-(3-hydroxy-3-methyl-1-buten-1-yl)-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



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RN 864684-16-2 CAPLUS
CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

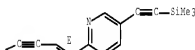
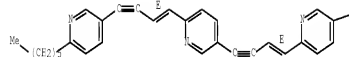


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RN 864684-06-0 CAPLUS
CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyne-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

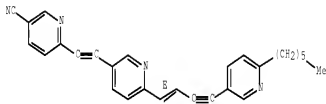


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RN 864684-17-3 CAPLUS

CN 3-Pyridinacarbonitrile, 6-[2-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]ethynyl]- (CA INDEX NAME)

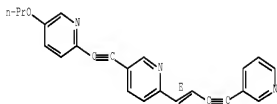
Double bond geometry as shown.



RN 864684-20-8 CAPLUS

CN Pyridine, 5-[2-[5-propoxy-2-pyridinyl]ethynyl]-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

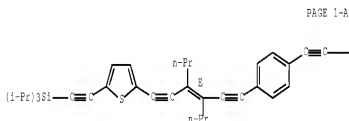
Double bond geometry as shown.



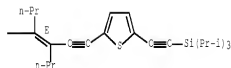
RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



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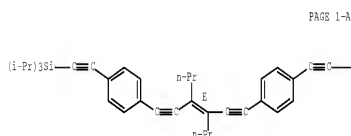


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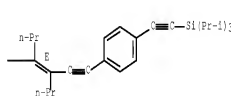
RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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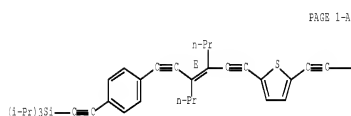


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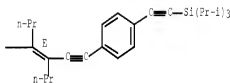
RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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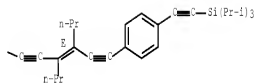


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RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diene-6,1-diyl]-4,1-phenylene-2,1-ethynadiyl]]bis[tris(1-methylethyl)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

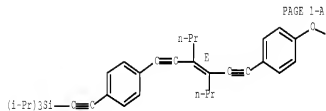


PAGE 1-B

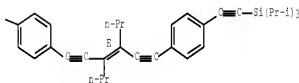
RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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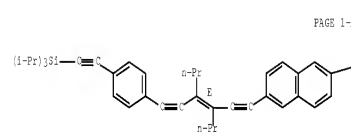


PAGE 1-B

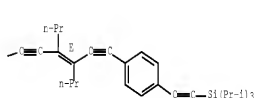
RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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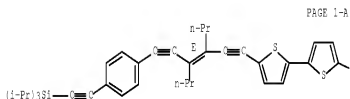


PAGE 1-B

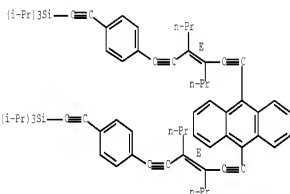
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

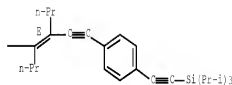
Double bond geometry as shown.



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RN 864684-30-0 CAPLUS

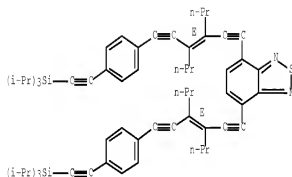
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

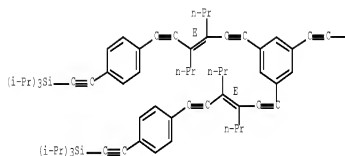
RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



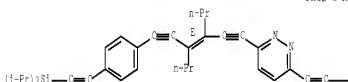
PAGE 1-A



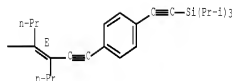
RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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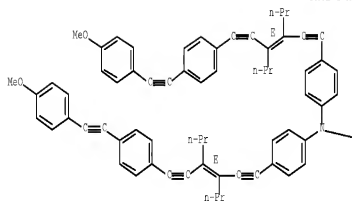
PAGE 1-B

RN 864684-33-3 CAPLUS

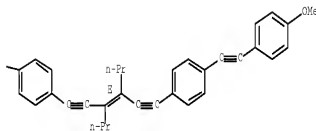
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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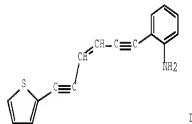


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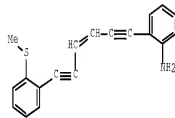


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN
 ACCESSION NUMBER: 2005:354187 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 143:333
 TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(2)-hexen-1,5-diyne, 2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their derivatives
 AUTHOR(S): Lin, Chi-Fong; Io, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Juh-Jeng; Wu, Ming-Jung
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:333



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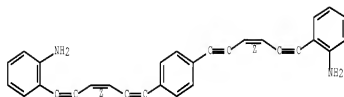


II

AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from <0.01 to 36.6 μ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10⁻⁷M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(2)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 852619:13:10
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(2)-hexen-1,5-diyne, 2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their derivs.)
 RN 852619-13-7 CAPLUS
 CN Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS
RECORD (15 CITINGS)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

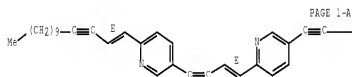
L7 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2004:832644 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 142:38113
TITLE: Site-Selective Monotitanation of Dialkynylpyridines
and Its Application for Preparation of Highly
Fluorescent π -Conjugated Oligomers
AUTHOR(S): Takayama, Yunki; Hanazawa, Takeshi; Andou, Tomohiro;
Miraoka, Kenji; Ohtani, Hiroyuki; Takahashi, Mizuki;
Sato, Fumie
CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo
Institute of Technology, Midori-ku, Yokohama,
Kanagawa, 226-8501, Japan
SOURCE: Organic Letters (2004), 6(23), 4253-4256
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:38113

AB Reaction of Ti(O-*i*-Pr)₄/2i-PrMgCl reagent with 2,*n*-
bis[(trimethylsilyl)ethynyl]pyridines, where *n* is 3, 4, 5, and 6, or with 3,4-
bis[(trimethylsilyl)ethynyl]pyridines, proceeded with excellent site-
selectivity to afford the corresponding monotitanated complex. Synthetic
application of the reaction was demonstrated by an efficient preparation of π -
conjugated oligomers having pyridine and enyne units alternately, which
possess intense blue fluorescence emission. Thus, reaction of 2,3-
bis[(trimethylsilyl)ethynyl]pyridine with Ti(O-*i*-Pr)₄/2i-PrMgCl reagent in
Et₂O gave 84% (2)-2-(2-(trimethylsilyl)ethynyl)-3-
[(trimethylsilyl)ethynyl]pyridine.

IT 805240-17-96 R09247-12-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
its preparation and site-selective monotitanation of dialkynylpyridines and
its application for preparation of highly fluorescent π -conjugated oligomers)

RN 805240-17-9 CAPLUS
CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-
yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

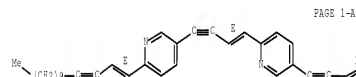


PAGE 1-A

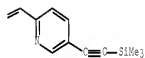
-SiMe3

RN 805240-18-0 CAPLUS
CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



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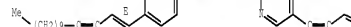


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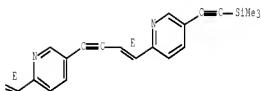
IT 805240-19-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and site-selective monotitanation of dialkynylpyridines and
its application for preparation of highly fluorescent π -conjugated oligomers)

RN 805240-19-1 CAPLUS
CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



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OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 2004:566840 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 141:261152
TITLE: π -Conjugated Dendrimers Based on
Bis(enediynyl)benzene Units
AUTHOR(S): Hwang, Gil Tae; Kim, Byeang Hyeon
CORPORATE SOURCE: National Research Laboratory, Department of Chemistry,
Division of Molecular and Life Sciences, Pohang
University of Science and Technology, Pohang, 790-784,
S. Korea

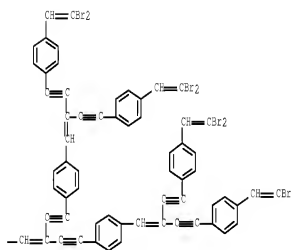
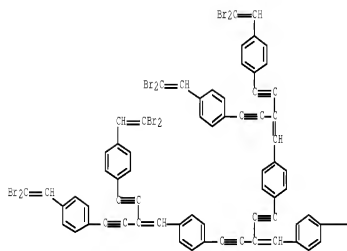
SOURCE: Organic Letters (2004), 6(16), 2669-2672
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have synthesized a new family of π -conjugated dendrimers that are based on
bis(enediynyl)benzene units by using both divergent and convergent approaches.
The comps. at all three generations have strong bluish-green fluorescence,
especially the third-generation dendrimer, which has the highest extinction
coefficient and quantum efficiency in this series.

IT 754233-16-4P 754233-18-6U
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(convergent and divergent synthesis of π -conjugated dendrimers based
on bis(enediynyl)benzene units)

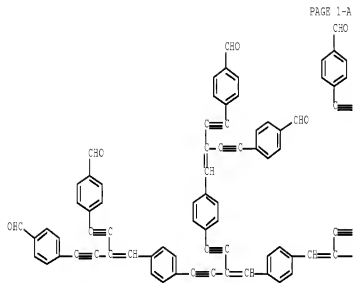
RN 754233-16-4 CAPLUS

CN Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-
dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-(4-(2,2-
dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-
ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

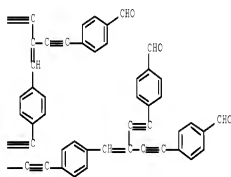


RN 754233-18-6 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-(4-(4-(4-formylphenyl)-2-[[4-
formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-(4-(4-formylphenyl)-2-
[[4-formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-
ynyl]phenyl]methylene)-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene[3-[[4-
formylphenyl]ethynyl]-3-buten-1-yn-4,1-diyl]]]]bis- (9CI) (CA INDEX NAME)



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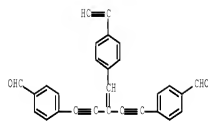


IT 206181-75-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(In convergent approach; convergent and divergent synthesis of
 π -conjugated dendrimers based on bis(enediynyl)benzene units)

RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-
diyl]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS
RECORD (17 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 13 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:490115 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and
Enediyne Units Alternately in the Backbone that Show
Intense Fluorescence Emission

AUTHOR(S): Makano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji;
Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo
Institute of Technology, Midori, Yokohama, Kanagawa,
226-8501, Japan

SOURCE: Organic Letters (2004), 6(14), 2373-2376

CODEN: ORLEF7; ISSN: 1523-7060

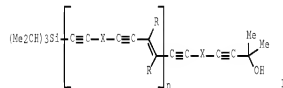
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

GI



AB Synthesis and fluorescence properties of π -conjugated compds. 1 ($n = 1 - 3$; X
= 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having
alternately an aromatic or heteroarom. ring and an enediyne unit in the
backbone are described.

IT 740610-61-1P 747317-62-2P 740810-63-3P

747317-65-5P 740810-63-7P 740610-66-8P

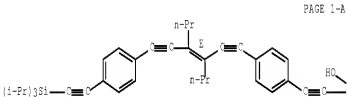
RL: PPP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(preparation and absorption and fluorescence spectra of conjugated
oligomers

having aromatic (or heteroarom.) and enediyne units alternately in the
backbone)

RN 740810-61-1 CAPLUS
CN 3-Butyn-2-ol, 2-methyl-4-[[4-[(3E)-3-propyl-4-[[2-4-[[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

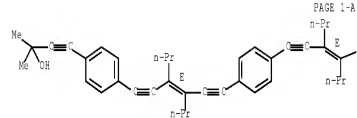


PAGE 1-B

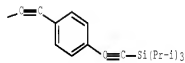


RN 740810-62-2 CAPLUS
CN 3-Butyn-2-ol, 2-methyl-4-[[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

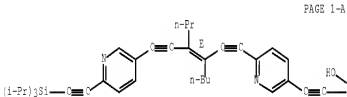


PAGE 1-B



RN 740810-64-4 CAPLUS
CN 3-Butyn-2-ol, 4-[[6-[(3E)-3-butyl-4-[[2-6-[[2-[[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

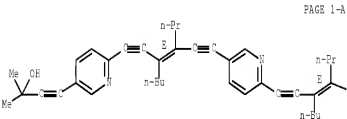


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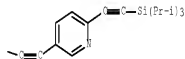


RN 740810-65-5 CAPLUS
CN 3-Butyn-2-ol, 4-[[6-[(3E)-3-butyl-4-[[2-6-[(3E)-3-butyl-4-[[2-6-[[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



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RN 740810-67-7 CAPLUS

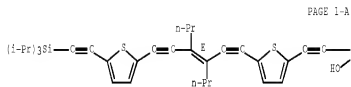
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

[[3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B

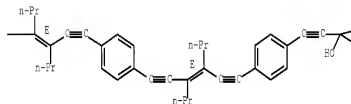


RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

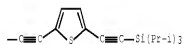
PAGE 1-B



PAGE 1-C



PAGE 1-B

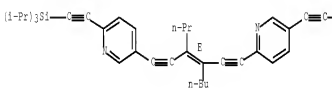


RN 740810-66-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

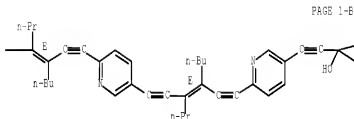


IT 740810-63-3E 740810-66-6P 740810-69-3P

RL: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

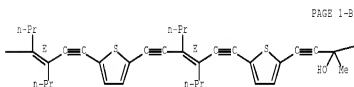
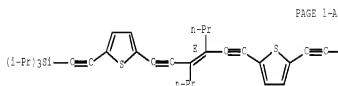
RN 740810-63-3 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-



RN 740810-69-9 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

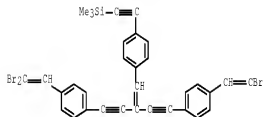
Double bond geometry as shown.



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2009 ACS on SIN
ACCESSION NUMBER: 2004:392953 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 141:88772
TITLE: Electrochemical and theoretical study of a family of fully conjugated dendritic oligomers
AUTHOR(S): Osorio, Gabriela; Frontana, Carlos; Guadarrama, Patricia; Frontana-Urbibe, Bernardo A.
CORPORATE SOURCE: Instituto de Química, UNAM, Circuito Exterior Ciudad Universitaria, Mexico, 04510, Mex.
SOURCE: Journal of Physical Organic Chemistry (2004), 17(5), 439-447
CODEN: JPOCEJ; ISSN: 0894-3230
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Novel dendritic oligomers of β,β -dibromo-4-ethynylstyrene and formyl-4-ethynylstyrene were electrochem. and theor. studied to gain a better insight into their redox behavior. Correlations between calculated ionization and expl. oxidation potentials (anodic peak potentials) were established. The best correlation was obtained when two important effects are considered in the theor. calcs., probing their strong influence: (a) structural re-accommodation in the formed radical cation and (b) solvation effects. The effect of dendritic terminal groups (dibromovinyl and formyl groups) was also analyzed. A different redox behavior was observed for these two terminal groups, presumably due to a difference in their oxidation mechanisms. A global chemical transformation for the oxidation of dibromovinyl-terminated oligomers was proposed, providing a satisfactory explanation of the electrochem. behavior within this family of (presence of adsorptive phenomena). Taking these results into account, it is possible to explain how the cation-radical species formed in these conjugated dendritic oligomers behave when cyclic voltammetry technique is applied.
IT 716327-63-8 716327-70-1 716327-91-2
RI: CFS (Chemical process); FMO (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (electrochem. and theor. study of fully conjugated dendritic oligomers family)

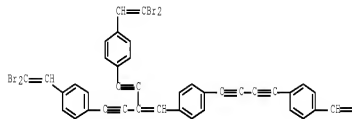
RN 716327-89-8 CAPLUS
CN Silane, [[4-(4-(4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (9CI) (CA INDEX NAME)



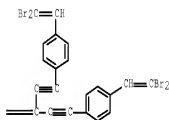
RN 716327-90-1 CAPLUS

CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(4-(2,2-dibromoethyl)phenyl)-2-[[4-(2,2-dibromoethyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1+) (SCI) (CA INDEX NAME)

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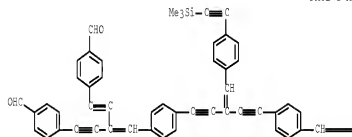
PAGE 1-B



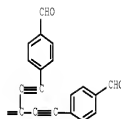
RN 716327-91-2 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-[[[trimethylsilyl]ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene(3-[[4-formylphenyl]ethynyl]]-3-buten-1-yne-4,1-diyl)]]bis-, radical ion(1+) (SCI) (CA INDEX NAME)

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IT 206181-74-0 206181-74-0 206181-76-0

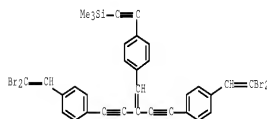
RI: CFS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(electrochem. and theor. study of fully conjugated dendritic oligomers family)

RN 206181-72-8 CAPLUS

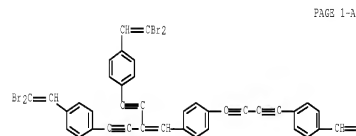
CN Silane, [[4-[4-(4-(2,2-dibromoethyl)phenyl)-2-[[4-(2,2-dibromoethyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-

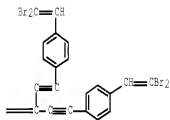
(9CI) (CA INDEX NAME)



RN 206181-74-0 CAPLUS

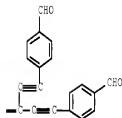
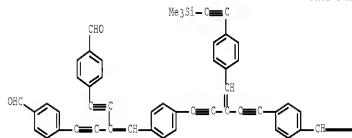
CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(4-(2,2-dibromoethyl)phenyl)-2-[[4-(2,2-dibromoethyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)





RN 206181-76-2 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-((trimethylsilyl)ethynyl)phenyl]methylene]-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene-3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



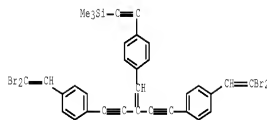
II 717144-23-5 717144-24-6 717144-25-7

RL FMO (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(electrochem. and theor. study of fully conjugated dendritic oligomers family)

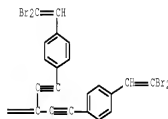
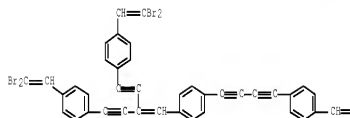
RN 717144-23-5 CAPLUS

CN Silane, [[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1-) (9CI) (CA INDEX NAME)



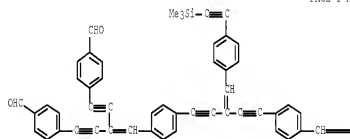
RN 717144-24-6 CAPLUS

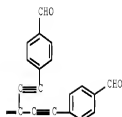
CN Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1-) (9CI) (CA INDEX NAME)



RN 717144-25-7 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-((trimethylsilyl)ethynyl)phenyl]methylene]-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene-3-[[4-formylphenyl]ethynyl]]-3-buten-1-yne-4,1-diyl]]bis-, radical ion(1-) (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 2004:328526 CAPLUS Full-text
DOCUMENT NUMBER: 141:54000
TITLE: Solid-phase synthesis of oligo(triacetylene)s and
oligo(phenylenetriacetylene)s employing Sonogashira
and Cadot-Chodkiewicz-type cross-coupling reactions
AUTHOR(S): Utesch, Nils F.; Diederich, Francois; Boudon, Corinne;
Glisselbrecht, Jean-Paul; Gross, Maurice
CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg,
HCI, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718
CODEN: HRCAGV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:54000

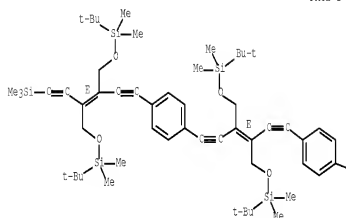
AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse
oligomers is described, using Pd0-catalyzed Sonogashira and Cadot-
Chodkiewicz-type cross-couplings as the key steps in the construction of the
acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-
iodoaryl)triazane linker was chosen as the polymeric support. The linker
selection was made based on the results of several model studies in the liquid
phase. For the solid-support synthesis of p-
1[CH4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 [I, n =
2-4] a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira
cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii)
cleavage of the linker with liberation of I. The longest-wavelength absorption
maxima of I [n = 1-4] shift bathochromically with increasing oligomeric
length, from λ_{max} 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the
electronic absorption data, the effective conjugation length (ECL) of the
oligo(phenylene triacetylene)s is estimated to involve at least four monomer
units and 40 C-atoms. π -Electron conjugation in these oligomers is less
efficient than in
Me3Si[CH4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 (II)
due to poor transmittance of π -electron delocalization by the Ph rings

inserted into the oligomeric backbone. Similar conclusions were drawn from
the electrochem. properties of the two oligomeric series as determined by
cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are
strongly fluorescent, with the highest quantum yield Φ_F = 0.69 measured for I
[n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded
smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions
employing Pd0-catalyzed Cadot-Chodkiewicz conditions still remain to be
developed.

IT 554459-52-02 554459-63-16 554459-64-22
RI: PREP (Properties); SYN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of oligo(triacetylene)s and
oligo(phenylenetriacetylene)s by Sonogashira and Cadot-Chodkiewicz
cross-coupling reactions)
RN 554459-62-0 CAPLUS
CN 4,9-Dioxo-3,10-disilaadodec-6-ene, 6-([4-[(3E)-3,4-bis{[(1,1-
dimethylethyl]dimethylsilyl]oxy)methyl]-6-(4-iodophenyl)-3-hexene-1,5-
diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-
[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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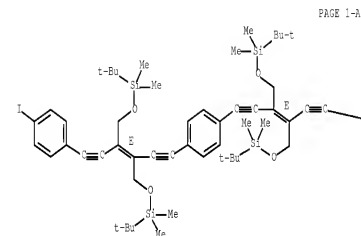


PAGE 1-B

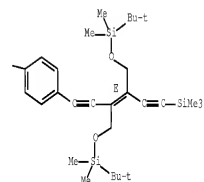
RN 554459-63-1 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[(4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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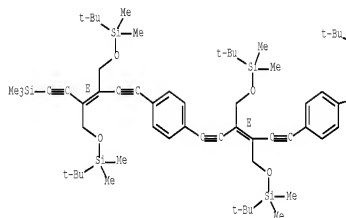


RN 554459-64-2 CAPLUS

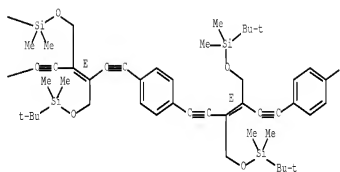
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[(4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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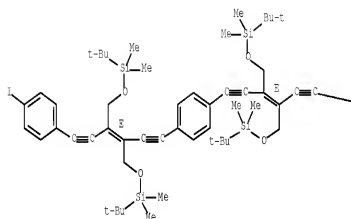
IT 704916-23-7P

RL: SPH (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadot-Chodkiewicz cross-coupling reactions)

RN 704916-29-0 CAPLUS

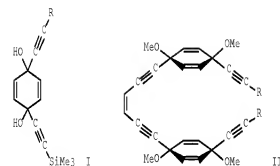
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[[4-(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)
REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN
ACCESSION NUMBER: 2003:491916 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 139:395637
TITLE: Synthesis of differentially protected/functionalised
acetylenic building blocks from p-benzoquinone and
their use in the synthesis of new enediynes
AUTHOR(S): Sankararaman, Seturaman; Srinivasan, Manivannan
CORPORATE SOURCE: Department of Chemistry, Indian Institute of
Technology Madras, Madras, 600 036, India
SOURCE: Organic & Biomolecular Chemistry (2003), 1(13),
2388-2392
CODEN: OBCHAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:395637
GI



AB Sequential addition of two different lithium acetylides to p-benzoquinone
yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4- diols I
[R = (Me2CH)3Si, (EtO)2CH] with different protective/functional groups on the
two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to
the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with
(Z)-1,2-dichloroethene yielded new enediynes II bearing cyclohexa-2,5-diene
units.

IT 626235-00-3P

RL: RCT (Reactant); SEN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

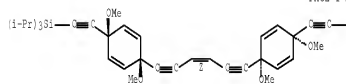
(preparation of cyclohexadienyl enediynes via double addition of
functionalized

lithium acetylides to benzoquinones, selective monodeprotection and
coupling with dichloroethene)

RN 626235-20-3 CAPLUS

CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diyl]bis[(cis-1,4-dimethoxy-2,5-
cyclohexadiene-1,4-diyl)-2,1-ethynediyl]bis[tris(1-methylethyl)- (3CI)
(CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



IT 626235-21-00 626235-22-1P

RL: SEN (Synthetic preparation); PREP (Preparation)
(preparation of cyclohexadienyl enediynes via double addition of
functionalized

lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethene)
 RN 626235-21-0 CAPLUS
 CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-(3,3-diethoxy-1-propynyl)-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry as shown.



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RN 626235-22-1 CAPLUS
 CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-ethynyl-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry as shown.

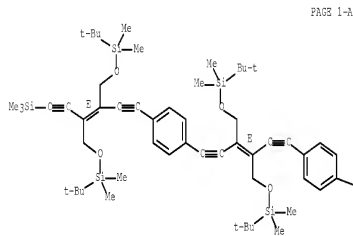


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 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 17 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STM
 ACCESSION NUMBER: 2003:234291 CAPLUS [Full-Text](#)
 DOCUMENT NUMBER: 139:85055
 TITLE: Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions
 AUTHOR(S): Utesch, Nils F.; Diederich, Francois
 CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Bonjgerberg, HCI, Zurich, CH-8093, Switz.
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 231-239
 CODEN: OBCHAK; ISSN: 1477-0520
 PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:85055
 AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., 1[4-C6H4C.tplbond.CCR.CCR.tplbond.C]nSiMe3 (R = C6H2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly π -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.
 IT 554459-62-0 554459-63-1P 554459-64-2P
 RL: FRP (Properties); SFN (Synthetic preparation); PREP (Preparation) (electronic absorption and emission, UV/VIS spectra; poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)
 RN 554459-62-0 CAPLUS
 CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-([4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(4-iodophenyl)]-3-hexene-1,5-diynyl]phenyl]ethynyl)-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



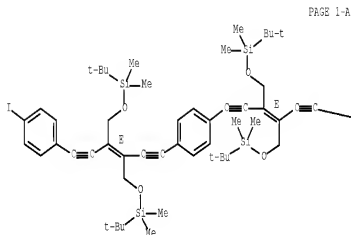
PAGE 1-A

PAGE 1-B

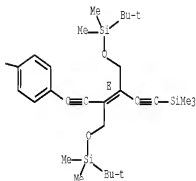
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RN 554459-63-1 CAPLUS
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-(4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,11,11-octamethyl-7-(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



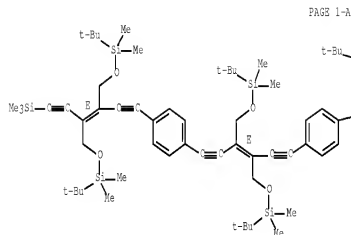
PAGE 1-A



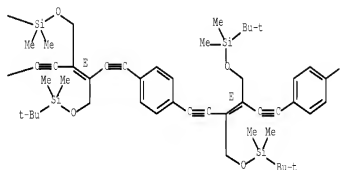
PAGE 1-B

RN 554459-64-2 CAPLUS
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-(4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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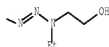
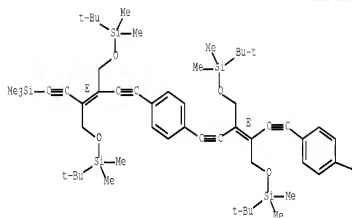


PAGE 1-B

IT 554459-71-10E, Merrifield resin-supported
 554459-72-20P, Merrifield resin-supported 554459-73-30P
 , Merrifield resin-supported
 RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed
 cross-coupling reactions of supported poly(triacetylene)-derived
 oligomers)

RN 554459-71-1 CAPLUS
 CN Ethanol, 2-[3-[4-[(3E)-6-(4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

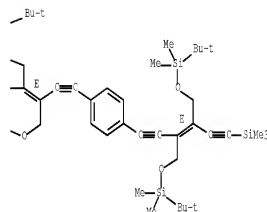
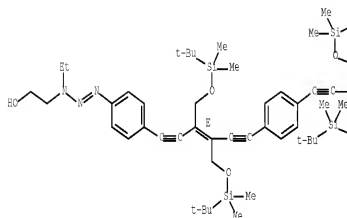
Double bond geometry as described by E or Z.



RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

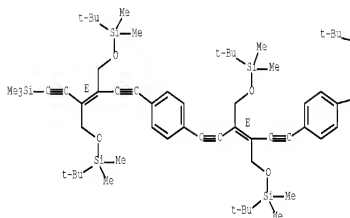


RN 554459-73-3 CAPLUS

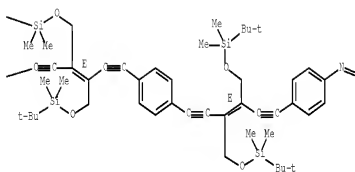
CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-6-[4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

DOCUMENT NUMBER: 137:208374
TITLE: Manufacturing method of semiconductor device using mask pattern having high etching resistance
INVENTOR(S): Otuchii, Junzo; Sato, Yasuhiko; Shiobara, Eishi; Hayashi, Hisataka; Ohwa, Tokuhisa; Onishi, Yasunobu
PATENT ASSIGNEE(S): Kabushiki Kaisha Toshiba, Japan
SOURCE: U.S. Pat. Appl. Publ., 26 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:



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PAGE 1-C

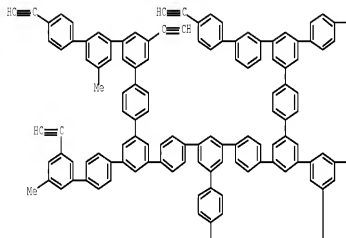


OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS
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REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

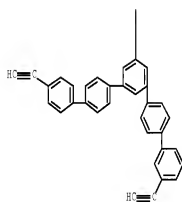
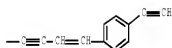
L7 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2002:658690 CAPLUS Full-text

PAGE 1-2





PAGE 1-B



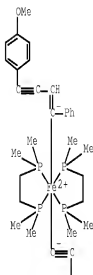
AB The acetylido Me iron(II) complexes, *cis/trans*-[Fe(dmpe)₂(C.tplbond.CR)(CH₃)] (1) and *trans*-[Fe(dmpe)₂(C.tplbond.CR)(CH₃)] (2) (dmpe = 1,2-dimethylphosphinoethane; depe = 1,2-diethylphosphinoethane), were synthesized by transmetalation from the corresponding alkyl halide complexes. Acetylido Me iron(III) complexes were also formed by transmetalation from the chloride complexes, *trans*-[Fe(dmpe)₂(C.tplbond.CR)(Cl)] or *trans*-[Fe(depe)₂(C.tplbond.CR)(Cl)]. The structure of *trans*-[Fe(dmpe)₂(C.tplbond.CC6H5)(CH₃)] (1a) was determined by single-crystal x-ray diffraction. The Me acetylido iron complexes, [Fe(dmpe)₂(C.tplbond.CR)(CH₃)] (1), are thermally stable in the presence of acetylenes; however, under UV irradiation, methane is lost with the formation of a metal bisacetylido. Photochem. metathesis of *cis*- or *trans*-[Fe(dmpe)₂(CH₃)(C.tplbond.CR)] [R = C₆H₅ (1a), 4-C₆H₄OCH₃ (1b)] with terminal acetylenes was used to selectively synthesize unsym. substituted iron(II) bisacetylido complexes of the type *trans*-[Fe(dmpe)₂(C.tplbond.CR)(C.tplbond.CR')]⁺ [R = Ph, R' = Ph (6a), 4-CH₃OC₆H₄ (6b), tBu (6c), SiMe₃ (6d), (CH₂)₄C.tplbond.CR (6e); R = 4-CH₃OC₆H₄, R' = 4-CH₃OC₆H₄, (6g), tBu (6h), (CH₂)₄C.tplbond.CR (6i), adamantyl (6j)]. The structure of the unsym. iron(II) bisacetylido complex *trans*-[Fe(dmpe)₂(C.tplbond.CC6H5)(C.tplbond.CC6H₄OCH₃)] (6b) was determined by single-crystal x-ray diffraction. The photochem. metathesis of the bisacetylene, 1,7-octadiyne, with *trans*-[Fe(dmpe)₂(CH₃)(C.tplbond.CPh)] (1a), was utilized to synthesize the bridged binuclear species *trans*-[C₆H₅C.tplbond.C][Fe(dmpe)₂(μ-C.tplbond.C)(CH₂)₄C.tplbond.C][Fe(dmpe)₂(C.tplbond.CC6H5)] (11). The trinuclear species *trans,trans,trans*-[C₆H₅C.tplbond.C][Fe(dmpe)₂(μ-C.tplbond.C)(CH₂)₄C.tplbond.C][Fe(dmpe)₂(μ-C.tplbond.C)(CH₂)₄C.tplbond.C][Fe(dmpe)₂(C.tplbond.CC6H5)] (12) was synthesized by the photochem. reaction of Fe(dmpe)₂(C.tplbond.CPh)(C.tplbond.C)(CH₂)₄C.tplbond.CE (6e) with Fe(dmpe)₂(CH₃)₂. Extended irradiation of the bisacetylido complexes with phenylacetylene resulted in insertion of the terminal alkyne into one of the metal acetylido bonds to give acetylido butynene complexes. The structure of the acetylido butynene complex, *trans*-[Fe(dmpe)₂(C.tplbond.CC6H₄OCH₃)(η¹-C(C6H5)CH(C.tplbond.CC6H₄OCH₃))] (3a) was determined by single-crystal x-ray diffraction.

IT 425380-70-7?
RL: PRP (Properties); SW (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 425380-70-7 CAPLUS
CN Iron, bis[1,2-ethanedithiolbis(dimethylphosphine-KF)]{[(4-methoxyphenyl)ethynyl][(1E)-4-(4-methoxyphenyl)-1-phenyl-1-butan-3-ynyl]-, (OC-6-1)-}-(9CI) (CA INDEX NAME)

06.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

L7 ANSWER 19 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 2002:198497 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 136:401857
TITLE: Acetylido-Bridged Organometallic Oligomers via the Photochemical Metathesis of Methyl-Iron(III) Complexes
AUTHOR(S): Field, Leslie D.; Turnbull, Anthony J.; Turner, Peter
CORPORATE SOURCE: School of Chemistry, The University of Sydney, Sydney, 2006, Australia
SOURCE: Journal of the American Chemical Society (2002), 124(14), 3692-3702
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:401857

PAGE 1-A



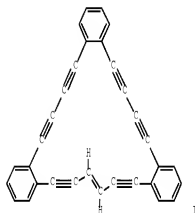
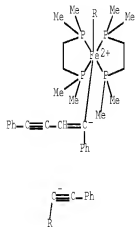
OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2009 ACS OR SIN
ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 136:69640
TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units
AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.
CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA
SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:69640
GI

PAGE 2-A



IT 426260-45-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 425380-85-4 CAPLUS
CN Iron, [(1E)-1,4-diphenyl-1-buten-3-ynyl]bis[1,2-ethanediyibis(dimethylphosphine-kP)] (phenylethynyl)-, (OC-6-11)-(9CI) (CA INDEX NAME)



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzenannulation.

IT 446260-17-4P 214628-18-8P 383404-36-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

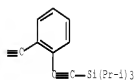
(preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)

PAGE 1-B

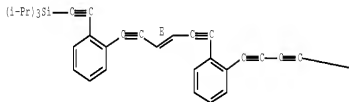
RN 214628-17-8 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[(3E)-6-(2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

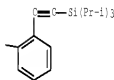
Double bond geometry as shown.



PAGE 1-A



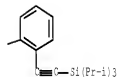
PAGE 1-B



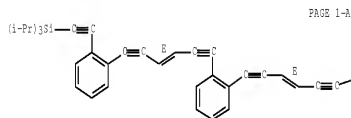
RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-(2-[[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

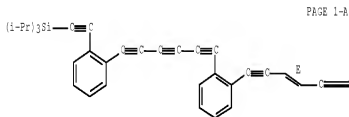


PAGE 1-B



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 2000:832492 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 134:310920
TITLE: Bis(enediynes) Macrocycles: Synthesis, Reactivity, and Structural Analysis
AUTHOR(S): Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.
CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA
SOURCE: Tetrahedron (2000), 56(49), 9581-9588
CODEN: TETNAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal



LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:310920

AB The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediyne) compds. The solid-state packing of one of the compds. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization

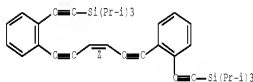
IT 335378-20-6P 335378-30-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bis(enediyne) macrocycles)

RN 335378-20-6 CAPLUS

CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

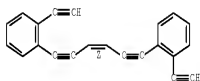
Double bond geometry as shown.



RN 335378-30-8 CAPLUS

CN Benzene, 1,1'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2-ethynyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:767122 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 134:71381

TITLE: Synthesis and structure of a new [6.6]metacyclophane with enediyne bridges

AUTHOR(S): Srinivasan, Manivannan; Sankararaman, Sethuraman; Dix, Ina; Jones, Peter G.

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, 600 036, India

SOURCE: Organic Letters (2000), 2(24), 3849-3851

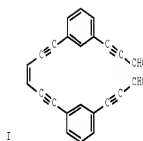
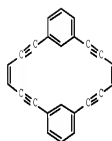
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:71381
GI



AB Synthesis and structure of a novel [6.6]metacyclophane with enediyne bridges I is reported. I was prepared by reacting 1,3-diethynylbenzene with EtMgBr/TEP and DMF to give the monoaldehyde. The monoaldehyde was subsequently converted to the acetal, coupled with ClCH₂CHCl₂ to give bis-acetal, which was hydrolyzed to the dialdehyde II. II underwent McMurry coupling using TiCl₃ and Zn-Cu couple in DME to give I in 69% yield.

IT 335378-30-6P 335378-31-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

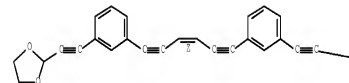
(preparation and crystal structure of metacyclophane with enediyne bridges)

RN 335378-30-6 CAPLUS

CN 1,3-Dioxolane, 2,2'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene-2,1-ethynediyl)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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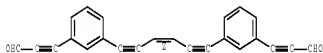
PAGE 1-B



RN 335378-31-7 CAPLUS

CN 2-Propynyl, 3,3'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1999:673316 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:337589

TITLE: Electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene

AUTHOR(S): Fomina, Serguei; Fomina, Lioudmila; Guadarrama, Patricia

CORPORATE SOURCE: Universidad Nacional Autonoma Mexico, Inst de Investigaciones en Materiales, Coyocacan, 04510 CU, Mex.

SOURCE: THEOCHEM (1999), 468, 207-216

CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Quantum-mech. calcs. of fully conjugated dendritic oligomers carried out at BLYP/3-21G/HE/3-21G (d) and BLYP/3-21G/PM3 levels of theory showed that loose dendritic architecture of β,β -dibromo-4-ethynyl styrene oligomers contributes little to the instability and conjugation disruption compared to 1 \rightarrow 2 branched polyacetylene, while Br terminal atoms in dendrimers strongly affect the electronic d. distribution in studied mols. On the one hand the bulky bromine atoms decrease the conjugation in Br-terminated dendrimers caused by steric hindrances, on the other hand, highly polarizable bromine atoms reduced significantly adiabatic ionization potentials (IPa) to be up to 1.5 eV lower than corresponding vertical potentials (IPv). Another phenomenon contributing to the reducing of IPa's of all dendrimers is the flattening of mol. geometry accompanying the ionization thus allowing better delocalization of pos. charge over the conjugated system while all aromatic ring except the very outer layer lost their aromaticity becoming essentially quinone by nature.

IT 206181-71-7 206181-72-3 206181-73-9

206181-74-0 206181-75-1 206181-76-2

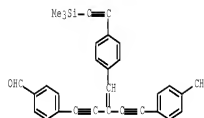
206181-77-3 206181-78-4 206181-79-5

RL: FRP (Properties)

(electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene)

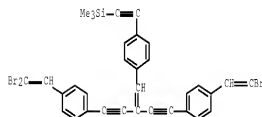
RN 206181-71-7 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiene-1,5-diyl]bis- (9CI) (CA INDEX NAME)



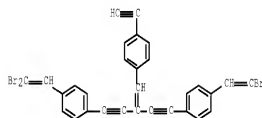
RN 206181-72-8 CAPLUS

CN Silane, [[4-[[4-[(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



RN 206181-73-9 CAPLUS

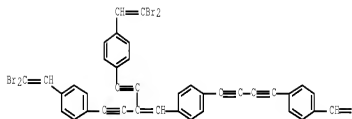
CN Benzene, 1,1'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiene-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)



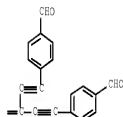
RN 206181-74-0 CAPLUS

CN Benzene, 1,1'-[1,3-butadiene-1,4-diyl]bis[4-[[4-[(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

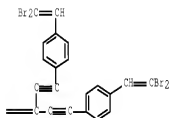
PAGE 1-A



PAGE 1-B



PAGE 1-B

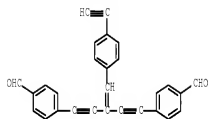


RN 206181-77-3 CAPLUS

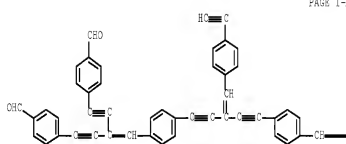
CN Benzaldehyde, 4,4'-[[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



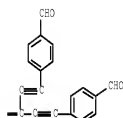
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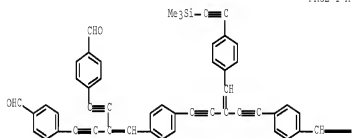
RN 206181-76-2 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-B



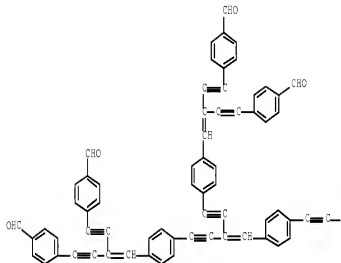
PAGE 1-A



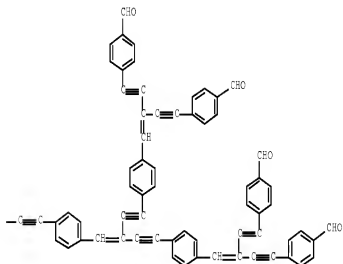
RN 206181-78-4 CAPLUS

CN Benzaldehyde, 4,4'-[[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-[[4-formylphenyl]-2-[[4-formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

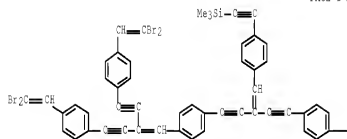
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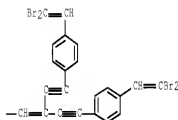
PAGE 1-B



PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 1999:650836 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 132:16702
TITLE: Theoretical description of luminescent effects in
 β,β -di(4'-formylphenylethynyl)-4-
ethynylstyrene
AUTHOR(S): Salcedo, R.; Guadarrama, P.; Sansores, L. E.; Fomina,
S.; Fomina, L.
CORPORATE SOURCE: Inst. de Investigaciones en Materiales, Inst. de
Investigaciones en Materiales, UNAM, Mexico, 04510,
Mex.
SOURCE: Materials Research Society Symposium Proceedings
(1999), 560 (Luminescent Materials), 359-364
CODEN: MRSFPH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English

RK 206181-79-5 CAPLUS
CN Silane, [[4-[[4-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-
dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[[4-(2,2-
dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-
ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trinechyl- (9CI) (CA
INDEX NAME)

AB Theor. calons. at HF/6-31 G(d) level were carried out on fully conjugated
comps. (4-ethynylbenzaldehyde, β,β -dibromo-4-ethynylstyrene, β,β -di(4'-
formylphenylethynyl)-4-ethynylstyrene and its dimer) to understand the source
of blue emission observed in oligomers of the 1st and 2nd generation in CHCl3
solns. The frontier orbitals are distributed through the framework of the
mols. (benzene rings, double and triple bonds and chromophores). Addnl., a CI
approach was applied over β,β -di(4'-formylphenylethynyl)-4-ethynylstyrene

(compound 3) at CIS/6-31 G(d) level to modeling excited states and simulate the UV-visible spectrum exptl. obtained. Calculated transitions corresponded to S0-S1 which are, presumably, responsible for the fluorescence observed

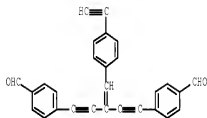
IT 206181-75-1 251479-84-2

RI: PRP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(theor. description of luminescent effects in styrene derivs.)

RN 206181-75-1 CAPLUS

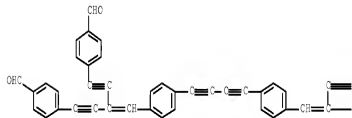
CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



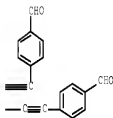
RN 251479-84-2 CAPLUS

CN Benzaldehyde, 4,4'-[1,3-butadiene-1,4-diylbis(4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 1998:756297 CAPLUS Full-text

DOCUMENT NUMBER: 130:118607

TITLE: Porphyrin-[(E)-1,2-diethynylethene] scaffolding. Synthesis and optical and electrochemical properties of multianometer-sized porphyrin arrays

AUTHOR(S): Wytko, Jennifer; Berl, Volker; Mclaughlin, Mark; Tykewski, Rik R.; Schreiber, Martin; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium Organische Chemie, STZ-Zentrum, Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (1998), 81(11), 1964-1977

CCDEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta AG

DOCUMENT TYPE: Journal

LANGUAGE: English

CI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two series of linearly conjugated hybrid materials, consisting of (E)-1,2-diethynylethene (DEE; hex-3-ene-1,5-diyne) and Zn(II) porphyrin components, were prepared by Pd0-catalyzed cross-coupling reactions. In I series, 1 or 2 DEE substituents were introduced into the meso-positions of the Zn(II) porphyrins, leading from Zn 3,15-bis[(ethoxycarbonyl)propoxy]phenylporphinate (I) to I and II (n = 1; R = SiMe2tBu). The second series contains the linearly x-conjugated mol. rods III (n = 1-3) that span a length range from 23 Å for III (n = 1) to 53 Å for III (n = 3). The larger rods III (n = 2 and 3) consist of 2 or 3 porphyrin moieties, resp., that are bridged at the meso-positions by trans-enediynediyl (hex-3-ene-1,5-diyne-1,6-diyl) linkers. The UV/Vis spectra in the series I, II, and III (n = 1) showed a strong bathochromic shift of both Soret and Q bands of the Zn(II) porphyrin as a result of the addition of DEE substituents. Upon changing from I to II, the Q band was further bathochromically shifted, whereas the Soret band remained nearly at the same position but became broadened and displayed a shoulder on the lower-wavelength edge as a result of excitonic coupling. The close resemblance between the UV/Vis spectra of III (n = 2 and 3) suggests that saturation of the optical properties in the oligomeric series already occurs at the stage of dimeric III (n = 2). Stationary voltammetric investigations showed that the DEE substituents act as strong electron acceptors which induce large anodic shifts in the 1st reduction potential upon changing from I to II (ΔE = 190 mV) and to III (n = 1) (ΔE = 340 mV). Increasing the number of porphyrin moieties upon changing from III (n = 1) to III (n = 2) had no effect on the 1st reduction potential yet the 1st oxidation potential was substantially lowered (ΔE = 110 mV). Large differences in the potentials for 1-electron oxidation of the 2 porphyrin moieties in III (n = 2) (ΔE = 200 mV) confirmed the existence of substantial electronic communication between the 2 macrocycles across the trans-enediynediyl bridge.

IT 219483-19-9

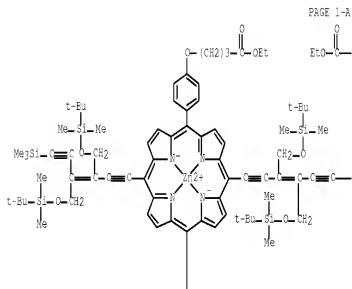
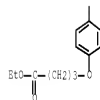
RI: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, UV spectra, electrochem. redox behavior and conversion to trinuclear complex and NMR)

RN 219483-19-9 CAPLUS

CN Zinc, [μ-[[tetraethyl 4,4',4'',4'''-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyne-1,6-diyl]bis[[20-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyne]-21H,23H-porphina-10,5,15-triyl-KN21,KN22,KN23,KN24]-4,1-phenyleneoxy]]tetrakis[butanoato]](4-))]di- (9CI) (CA INDEX NAME)

PAGE 2-A



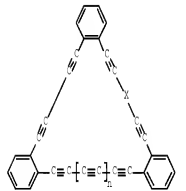
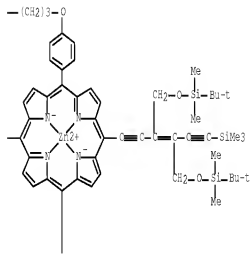
PAGE 1-A

PAGE 2-B



OS.CITING REF COUNT: 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2009 ACS or SIN
ACCESSION NUMBER: 1998:606810 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 129:302407
ORIGINAL REFERENCE NO.: 129:61683a,61686a
TITLE: Synthesis of expanded planar dehydrobenzocorroles: weakly diatropic, weakly paratropic, or atropic?
AUTHOR(S): Wan, W. Brad; Kimball, David B.; Haley, Michael M.
CORPORATE SOURCE: Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA
SOURCE: Tetrahedron Letters (1998), 39(38), 6795-6798
CODEN: TETLEA; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:302407
GI



AB Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes **1** [$X = \text{C, tpbond, C, (E)-CH=CH; } n = 0, 1$] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannulation, dehydrobenzoannulenes possess weak induced ring currents.

IT 214628-17-8P 214628-18-9P

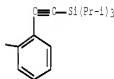
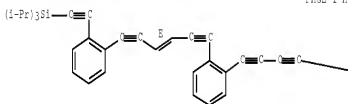
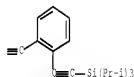
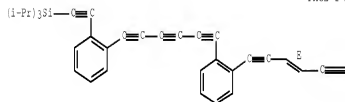
RU: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of expanded planar dehydrobenzoannulenes with triacetylenic linkages)

RN 214628-17-8 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

CS.CITING REF COUNT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:269262 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 128:257221

ORIGINAL REFERENCE NO.: 128:50919a,50922a

TITLE: Steric Hindrance Facilitated Synthesis of Enynes and Their Intramolecular [4 + 2] Cycloaddition with Alkynes

AUTHOR(S): Gonzalez, Juan J.; Francesch, Andres; Cardenas, Diego J.; Echavarren, Antonio M.

CORPORATE SOURCE: Departamento de Química Orgánica, Universidad Autónoma de Madrid, Madrid, 28049, Spain

SOURCE: Journal of Organic Chemistry (1998), 63(9), 2854-2857
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:257221

AB The palladium-catalyzed insertion of 1-alkynes into internal alkynes which are bent out of linearity by the interference with a peri or ortho substituent led to enynes regioselectively. The resulting enynes undergo a new type of intramolecular thermal cycloaddition, which can be used for the annulation of an aryl ring onto naphthalene derivatives to afford fluorenones. The cyclization of (E)-1-[(1-buten-3-ynyl)-8-ethynyl]naphthalene could also be performed in the presence of a Cu(I) catalyst at room temperature

IT 205124-39-6P

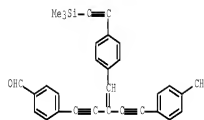
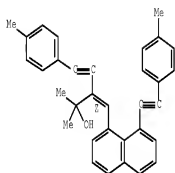
RU: SPN (Synthetic preparation); PREP (Preparation)

(preparation of enynes and their intramolecular [4+2] cycloaddition with alkynes)

RN 205124-39-6 CAPLUS

CN 4-Pentyn-2-ol, 2-methyl-5-(4-methylphenyl)-3-[[8-[2-(4-methylphenyl)ethynyl]-1-naphthalenyl]methylene]-, (3Z)- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

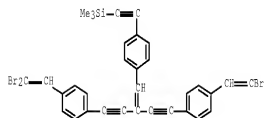
L7 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 1998:247633 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 128:295129
ORIGINAL REFERENCE NO.: 128:58501a,58504a
TITLE: Synthesis and characterization of well-defined fully conjugated hyperbranched oligomers of β,β -dibromo-4-ethynylstyrene
AUTHOR(S): Fomina, Lioudmila; Guadarrama, Patricia; Fomine, Sarguis; Salcedo, Roberto; Ogawa, Takeshi
CORPORATE SOURCE: Instituto Investigaciones Materiales, Univ. Nacional Autonoma de Mexico, Mexico, 04510, Mex.
SOURCE: Polymer (1998), 39(12), 2629-2635
CODEN: POLMAG; ISSN: 0032-3861
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Well-defined dendritic oligomers of poly(β,β -dibromo-4-ethynylstyrene) of the first and second generation were synthesized by a stepwise synthesis, and characterized. NMR and theor. calcs. showed that free rotation around formal single bonds is hampered by conjugation. All of the oligomers were blue emitters with their emission maxima correlating with the number of repeating units. All dendrimers except β,β -bis[β,β' -di(β,β' -dibromostyryl)-4'-ethynyl]styryl-4'-ethynyl-4-ethynylstyrene showed two maxima in the excitation spectra.

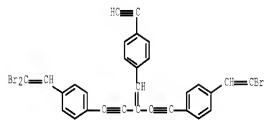
IT 206181-71-7R 206181-72-8R 206181-73-9P
206181-74-0P 206181-75-1P 206181-76-2P
206181-77-3P 206181-78-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PRP (Preparation); RACT (Reactant or reagent)
(preparation and characterization of conjugated hyperbranched β,β -dibromo-4-ethynylstyrene oligomers)

RN 206181-71-7 CAPLUS
CN Benzaldehyde, 4,4'-[3-[[4-[[trimethylsilyl]ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)

RN 206181-72-8 CAPLUS
CN Silane, [[4-[4-(4-(2,2-dibromoethenyl)phenyl]phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)

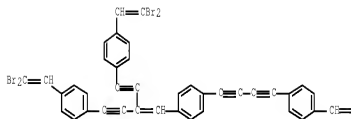


RN 206181-73-9 CAPLUS
CN Benzene, 1,1'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)

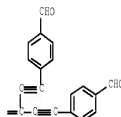


RN 206181-74-0 CAPLUS
CN Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

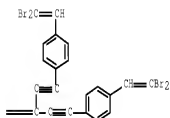
PAGE 1-A



PAGE 1-B

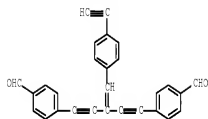


PAGE 1-B

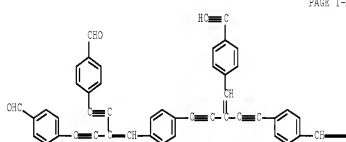


RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



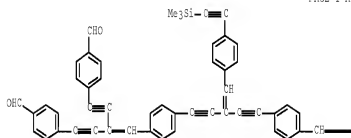
PAGE 1-A



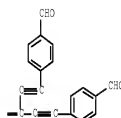
RN 206181-76-2 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

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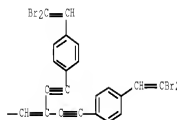
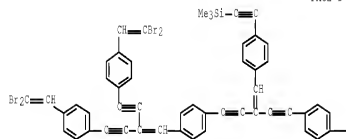
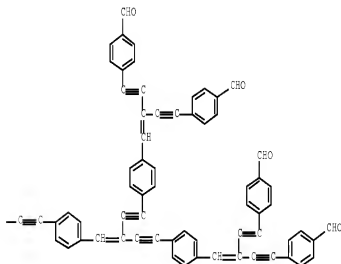
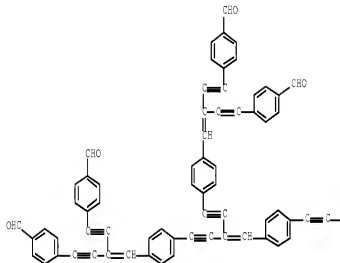


PAGE 1-B



RN 206181-78-4 CAPLUS

CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis(4,1-phenylene[3-[[4-(4-formylphenyl)-2-[[4-(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[[4-(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)
 REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

17 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:303100 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 125:11582
 ORIGINAL REFERENCE NO.: 125:2539a,2542a
 TITLE: Synthesis and polymerization of

β , β -dibromo-4-ethynylstyrene; preparation of a new polyconjugated, hyperbranched polymer

AUTHOR(S): Fomina, Lioudmila; Salcedo, Roberto
 CORPORATE SOURCE: Inst. Investigaciones Materiales, Circuito Exterior, Ciudad Univ., Mexico City, 04510, Mex.
 SOURCE: Polymer (1996), 37(9), 1723-1728
 CODEN: POLMAG; ISSN: 0032-3861

PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The monomer, β , β -dibromo-4-ethynylstyrene, was prepared and polymerized by the Heck reaction to give a partially soluble, conjugated hyperbranched polymer. The polymer structure was elucidated using standard spectroscopic techniques and with the aid of model compound synthesis. Theor. calcs. using the AM1 method were carried out and showed that conjugation in the polymer is partially disrupted by twisting of the benzene rings. Both the model compound and the polymer showed luminescence.

IT 177410-69-1P

RL: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

IT 206181-79-5P

RL: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and characterization of conjugated hyperbranched β , β -dibromo-4-ethynylstyrene oligomers)

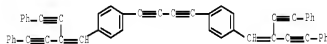
RN 206181-79-5 CAPLUS

CN Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)

(model compound for dibromoethynylstyrene polymer)

RN 177410-40-1 CAPLUS

CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-(4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl)]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L7 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1995:94580 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 124:9540

ORIGINAL REFERENCE NO.: 124:2031a,2034a

TITLE: Novel polymers containing discrete conjugated units, produced by the Heck reaction
AUTHOR(S): Fomina, Sergei; Fomina, Lioudmila; Florentino, Hector Quirez; Mendez, Juan Manuel; Ogawa, Takeshi
CORPORATE SOURCE: Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Coyoacan, 04510, Mex.

SOURCE: Polymer Journal (Tokyo) (1995), 27(11), 1085-93

CODEN: POLUB8; ISSN: 0032-3896

PUBLISHER: Society of Polymer Science, Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

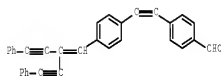
AB Novel monomers and polymers containing arylenevinylideneethynylene groups were synthesized via the Heck reaction. The polymers were amorphous and soluble in common organic solvents. They have T_g approx.60°, 5% weight loss at 240-240° and undergo thermal crosslinking at 170-190° with loss of triple bonds. One of the polymers exhibits strong blue luminescence with emission maxima approx.380-390 and 470-480 nm with excitation at 320 nm. All polymers show 3rd order MLO susceptibility approx.10-10 esu.

IT 171296-95-00

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Intermediate; in preparation of polyacetylene-polyesters)

RN 171296-95-0 CAPLUS

CN Benzaldehyde, 4-[2-[4-(4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl)phenyl]ethynyl]- (CA INDEX NAME)



IT 171296-96-1P

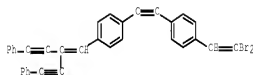
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(monomer; in preparation of polyacetylene-polyesters)

RN 171296-96-1 CAPLUS

CN Benzene, 1-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



IT 171296-99-4P

RL: PREP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, characterization and properties of)

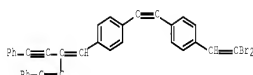
RN 171296-99-4 CAPLUS

CN Decanedioic acid, di-2-propynyl ester, polymer with 1-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-ynyl]benzene (9CI) (CA INDEX NAME)

CM 1

CRN 171296-96-1

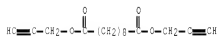
CMF C34 E20 Br2



CM 2

CRN 93164-22-8

CMF C16 E22 O4

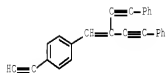


IT 171297-02-2, β,β -Bis(phenylethynyl)-4-ethynylstyrene

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; in preparation of polyacetylene-polyesters)

RN 171297-02-2 CAPLUS

CN Benzene, 1-ethynyl-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L7 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN
 ACCESSION NUMBER: 1995:642218 CAPLUS Full-text
 DOCUMENT NUMBER: 123:33763
 ORIGINAL REFERENCE NO.: 123:6259a,6262a
 TITLE: Synthesis and molten-state polymerization of some novel conjugated diacetylenes
 AUTHOR(S): Fomina, Lioudmila; Allier, Hector; Fomine, Sergel; Salcedo, Roberto; Ogawa, Takeshi
 CORPORATE SOURCE: Inst. Investigaciones Materiales, Ciudad Univ., Mexico, 04510, Mex.
 SOURCE: Polymer Journal (Tokyo) (1995), 27(6), 591-600
 CODEN: POLJ88; ISSN: 0032-3896
 PUBLISHER: Society of Polymer Science, Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English

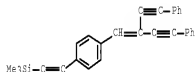
AB A series of new, highly conjugated diacetylenes, 4-ethynylstilbene derivs., was synthesized and their polymerization was studied. None of them was found to undergo topochem. polymerization in the solid state but they readily polymerized in the molten state to give red transparent and amorphous polymers. All the polymers had an absorption maximum in the visible spectra around 500 nm, and FT-IR data showed the enyne structure of the polymer chain resulted from 1,4-addition

IT 164467-30-16

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (in preparation of ethynylstilbene derivative monomers)

RN 164467-30-5 CAPLUS

CN Benzene, 1-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-4-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



IT 164467-25-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and characterization of polydiacetylenes from ethynylstilbene derivs. in molten state)

RN 164467-25-8 CAPLUS

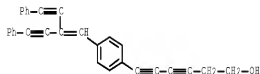
CN 3,5-Hexadiyn-1-ol, 6-[4-(4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl)phenyl]-

, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 164467-20-3

CME C30 E20 O

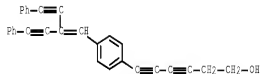


IT 164467-20-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and polymerization of)

RN 164467-20-3 CAPLUS

CN 3,5-Hexadiyn-1-ol, 6-[4-(4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L7 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 1994:522234 CAPLUS Full-text

DOCUMENT NUMBER: 121:122234

ORIGINAL REFERENCE NO.: 121:21825h,21826a

TITLE: Difluoride derivative and liquid crystal composition containing the same

INVENTOR(S): Yokokoji, Osamu; Irisawa, Jun; Koh, Hidenasa

PATENT ASSIGNEE(S): Asahi Glass Co., Ltd., Japan

SOURCE: PCT Int. Appl., 43 pp.

CODEN: F1XXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

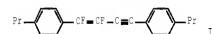
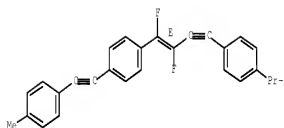
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405613	A1	19940317	WO 1993-UP1235	19930901
W: US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 628528	A1	19941214	EP 1993-919002	19930901

R: CE, FR, GB, IT
 JP 06263661 A 19940920 JP 1993-219709 19930903
 JP 3564711 B2 20040915
 US 5419851 A 19950530 US 1994-211625 19940420
 JP 2004292454 A 20041021 JP 2004-115211 20040409
 JP 3707493 B2 20051019
 PRIORITY APPLN. INFO.: JP 1992-263027 A 19920904
 WO 1993-TP1235 W 19930901
 JP 1993-219709 A3 19930903

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LUSIS DISPLAY FORMAT
 OTHER SOURCE(S): HARPAT 121:122234

G1



AB Difluoride derivs. represented by the general formula:
 $R1(A1Y1)2ACFC:CF:C.tplbond.CA3(Y2M4)nR2$ (A1 - A4 = trans-1,4-cyclohexylene, 1,4-cyclohexanylene, or 1,4-phenylene wherein 21 CH groups of each ring may be substituted by H or 21 CH2 groups of the ring may be substituted by O or S; m, n = 0, 1; R1, R2 = C1-10 alkyl, halo, cyano wherein (1) O, CO2, or O2C may be inserted between the C-C bond of alkyl or that between alkyl and ring, (2) a part of the C-C bonds in alkyl is replaced by C/C or C.tplbond.C bond, or (3) one CH2 group in alkyl is replaced by CO group; Y1, Y2 = CO2, COC, C.tplbond.C, CH2CH2, CH/CH, OCH2, CH2O) are prepared. These compds. have low viscosity, are light-stable, and hence can provide a liquid crystal composition having high response speed. Thus, 0.1 mol ClCF:CF2 was blown into THF at -100° followed by adding dropwise 62.1 mL 1.61 M BuLi/hexane, stirring for 30 min, adding dropwise 0.1 mol Me3SiCl, stirring for 1 h, adding dropwise a solution of 4-propylphenyl lithium in THF (prepared from 4-propyliodobenzene and BuLi) at -100°, and stirring for 2 h at 0° to give 75% (Z)-4-PrC6H4CF:CFSiMe3. The latter compound (0.075 mol) was reacted with 0.15 mol HF in aqueous MeCN at 70° for 1 h to give 83% (E)-4-PrC6H4CF:CFH which (0.062 mol) was dissolved in THF, cooled to -78°, and treated dropwise with 36.5 mL 1.61 M BuLi/hexane followed by stirring for 30 min, adding 15.7 g iodine, and stirring at room temperature for 4 h to give 83% (E)-4-PrC6H4CF:CFI. The latter compound (0.051 mol) and 0.051 mol 4-propylphenylacetylene were dissolved in 100 mL Et3N followed by adding Pd(PPh3)2Cl2 and CuI and the resulting mixture was allowed to react at room temperature for 5 h to give 70% diphenyldifluorobutane derivative (I). A STN-type liquid crystal display device was prepared from a liquid composition containing 20 weight% I and 80 weight% ZLI-1565 and irradiated with a UV carbon arc lamp for 200 h; new compds. were hardly formed whereas cis-4,4'-bis(n-propyl)difluorostilbene was formed in a liquid crystal composition containing ZLI-1565 and trans-4,4'-bis(n-propyl)difluorostilbene.

IT 158869-08-66
 RI: SPW (Synthetic preparation); PREP (Preparation)
 (preparation of, as liquid crystal with UV stability and low viscosity)
 RN 158869-08-8 CAPLUS
 CN Benzene, 1-[1,2-difluoro-4-(4-propylphenyl)-1-buten-3-ynyl]-4-[(4-methylphenyl)ethynyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Uploading C:\Program Files\STNEXP\Queries\10591950-claim-2-v 1.str



chain nodes :
 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
 chain bonds :
 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-16 16-17 17-18
 18-19 19-20
 exact/norm.bonds :
 4-5 5-6 11-12 12-13 18-19 19-20
 exact bonds :
 6-7 7-8 8-9 9-10 10-11 13-14 14-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,SI,Cb,Cy,Hy

Match level :

4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS

L8 STRUCTURE UPLOADED

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FULL SEARCH INITIATED 13:20:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 11728 TO ITERATE

100.04 PROCESSED 11728 ITERATIONS

70 ANSWERS

SEARCH TIME: 00.00.01

L9 70 SEA SSS FUL 18

=> file caplus

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L10 22 L9

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YOU HAVE REQUESTED DATA FROM 22 ANSWERS - CONTINUE? Y/(N):y

L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2009:1099083 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 151:508432

TITLE: Hybrid Conjugated Organic Oligomers Consisting of Oligodiacetylene and Thiophene Units: Synthesis and Optical Properties

PAGE 1-B

AUTHOR(S): Filizak, Gregor S.; van Gruithuysen, Kitty; van Doorn, Reinbert H.; van Lagen, Barend; Sothoelster, Ernst J. R.; Zuilhof, Han

CORPORATE SOURCE: Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, Wageningen, 6703 HB, Neth.

SOURCE: Chemistry--A European Journal (2009), 15(36),

9085-9096, S9085/1-S9085/19

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 151:508432

AB Novel and highly soluble hybrid conjugated organic oligomers consisting of oligodiacetylene and thiophene units have been synthesized in high purity through iterative and divergent approaches based on a sequence of Sonogashira reactions. The series of thiophene-containing oligodiacetylenes and homocoupled oligodiacetylenes show, both in solution and in the solid state, a strong optical absorption, which is progressively red shifted with increasing chain length. The linear correlation of the absorption maximum with the inverse of conjugation length (CL = number of double and triple bonds) shows that the effective conjugation length of this system is extended up to at least CL = 20. Furthermore, absorption measurements of dropcast thin films display not only a bathochronic shift of the absorption maxima but also a higher wavelength absorption, which is attributed to increased π - π interactions. The wavelength of the maximum fluorescence emission also increases with CL, and emission is maximal for oligomers with CL = 7-12 (fluorescence quantum yield Φ_F = .apprx.0.2). Both longer and shorter oligomers display marginal emission. The calculated Stokes shifts of these planar materials are relatively large (0.4 eV) for all oligomers, and likely due to excitation to the S2 state, thus suggesting that the presence of enyne moieties dominates the ordering of the lowest excited states. The fluorescence lifetimes (τ_F) are short (τ_{max} = <1 ns) and closely follow the

tendency obtained for the fluorescence quantum yield. The anisotropy lifetimes show a near-linear increase with CL in line with highly rigid oligomers.

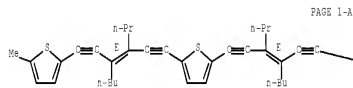
IT 1102820-73-3P

RI: FRP (Properties); SFM (Synthetic preparation); PREP (Preparation) (synthesis via iterative Sonogashira coupling and optical properties of hybrid conjugated organic oligomers consisting of oligodiacetylene and thiophene units)

RN 1192820-73-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2009:76616 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 150:167710

TITLE: Push-pull hyperbranched molecules. A theoretical study
AUTHOR(S): Ramos, Estrella; Guadarrama, Patricia; Taran, Gerardo; Fomina, Serguei

CORPORATE SOURCE: Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Mexico, 04510, Mex.

SOURCE: Journal of Physical Organic Chemistry (2009), 22(1), 9-16

CODEN: JPOCEJ; ISSN: 0894-3230

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electronic properties of the ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups have been studied at B3LYP/cc-pvdz//HF/6-31g(d), TD-B3LYP/cc-pvdz//HF/6-31g(d) and TD-B3LYP/cc-pvdz//CIS/6-31g(d) levels of theory, resp. It was demonstrated that dendritic architecture of push-pull mols. favors the charge transfer in the excited state compared to linear mols. The possibility of adopting a plane conformation is an important condition for the charge transfer in an excited state. According to the calcs. 1:1 ratio of donor and acceptor groups is another important precondition for the manifestation of

strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the $S_0 \rightarrow S_1$ transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

PAGE 1-B

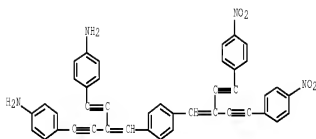
IT 1107616-70-5 1107616-72-7

RL: PPP (Properties)

(electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

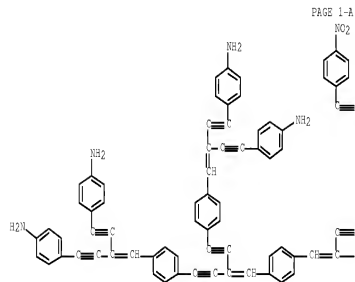
RN 1107616-70-5 CAPLUS

CN Benzenamine, 4,4'-[3-[[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

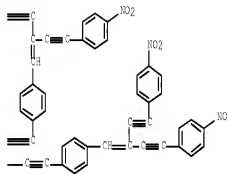


RN 1107616-72-7 CAPLUS

CN Benzenamine, 4,4'-[3-[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



PAGE 1-A



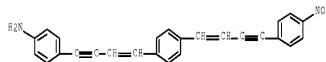
IT 1107616-75-0 1107616-76-1

RL: PPP (Properties)

(linear analog; electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

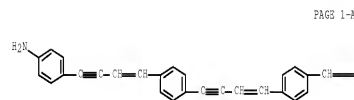
RN 1107616-75-0 CAPLUS

CN Benzenamine, 4-[4-[4-[4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

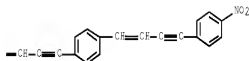


RN 1107616-76-1 CAPLUS

CN Benzenamine, 4-[4-[4-[4-[4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl]-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)



PAGE 1-A



CRN 1015477-29-8
CME C67 E56 B N7 O P2 Ru
CCI CCS

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 2008:244421 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:403337

TITLE: Triphenylphosphine Incorporation Reactions of Diynyl Complexes Containing a $\text{TpRu}(\text{NO})$ Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene
Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Kenta; Umakoshi, Keisuke; Onishi, Masayoshi

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan

SOURCE: Organometallics (2008), 27(6), 1227-1233

CODEN: ORGN07; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:403337

AB Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand ($\text{Tp} = \text{BH}[\text{pyrazol-1-yl}]_3$) were prepared, and their reactivities toward PPh_3 incorporation in the presence of $\text{HBF}_4 \cdot \text{Et}_2\text{O}$ were described. The PPh_3 incorporation of mono(arylbutadiynyl) complex $\text{TpRuCl}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{NO})$ (1) resulted in the β -phosphonoalkenyl complex $[\text{E}]-[\text{TpRuCl}(\text{CH}(\text{C}(\text{PPh}_3)-\text{C.tplbond.C-C6H4Me})(\text{NO}))\text{BF}_4]$ (2-BF4), whereas when his(arylbutadiynyl) $\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})_2(\text{NO})$ (3) was treated, mono- and his β -phosphonoalkenyl complexes $[\text{E}]-[\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{CH}(\text{C}(\text{PPh}_3)-\text{C.tplbond.C-C6H4Me})(\text{NO}))\text{BF}_4]$ (4-BF4) and $[\text{E,E}]-[\text{TpRu}(\text{CH}(\text{C}(\text{PPh}_3)-\text{C.tplbond.C-C6H4Me})_2(\text{NO}))\text{BF}_4]$ (5-BF4) were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutadiynyl) (3-hydroxyalkenyl) complex, $\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{C.tplbond.CCPH}_2(\text{OH}))(\text{NO})$ (6), was allowed to react with PPh_3 in the presence of the protic acid to give the α -phosphonoalkenyl $[\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{C}(\text{PPh}_3)(\text{C}(\text{CPH}_2)(\text{NO}))\text{BF}_4]$ (7-BF4). Interestingly, thermal isomerization of 7-BF4 to a ruthena-2- PPh_3 -cyclobuta[b]naphthalene $[\text{TpRu}(\text{CH}(\text{PPh}_3)(3\text{-Ph-8-(MeC6H4-C.tplbond.C-C10H4))(\text{NO}))\text{BF}_4]$ (8-BF4) was observed

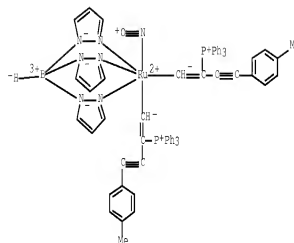
IT 1015477-59-1P

RU: SPN (Synthetic preparation); PREP (Preparation)

(triphenylphosphine incorporation reactions of diynyl complexes containing pyrazolylboratoruthenium nitrosyl fragment and isomerization to ruthenacyclobutanaphthalene)

RN 1015477-30-1 CAPLUS

CN Ruthenium(2+), [bicycrotis(18-pyrazolato- κN1)borato(1-)- $\kappa\text{N2}, \kappa\text{N2}''$][his(1E)-4-(4-methylphenyl)-2-(triphenylphosphino)-1-but-3-yn-1-yl]nitrosyl-, (OC-6-23)-, tetrafluoroborate(1-) (1:2) (CA INDEX NAME)



CRN 14874-70-5

CME B F4

CCI CCS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER: 2008:112838 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:331583

TITLE: 3-Iodo-3-trimethylsilylpropenal as a useful unit for pinacol coupling and subsequent functional group transformations

AUTHOR(S): Shimizu, Makoto; Okimura, Hisashi; Manabe, Nobuyuki; Hachiya, Iwao

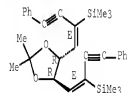
CORPORATE SOURCE: Department of Chemistry for Materials, Graduate School of Engineering, Mie University, Tsu, 514-8507, Japan
Chemistry Letters (2008), 37(1), 28-29

CODEN: CHLTJG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 148:331583
 AB Stereoselective titanium tetraiodide-promoted pinacol coupling reactions of (Z)-3-halo-3-(substituted-silyl)prop-2-en-1-als are used for the preparation of trans-4,5-bis[(Z)-2-halo-2-(substituted-silyl)vinyl]-2,2-dimethyl-1,3-dioxolanes. These dioxolanes are then used for subsequent C-C bond-forming reactions.
 IT 1611294-74-6P
 RU: SPW (Synthetic preparation); PRPP (Preparation)
 (3-halo-3-(substituted-silyl)prop-2-en-1-als are reactants for stereoselective pinacol coupling to form bis-substituted dioxolanes)
 RN 1011296-76-6 CAPLUS
 CN 1,3-Dioxolane, 2,2-dimethyl-4,5-bis[(E)-4-phenyl-2-(trimethylsilyl)-1-buten-3-yn-1-yl]-, (4R,5R)-rel- (CA INDEX NAME)

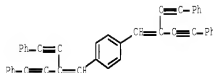
Relative stereochemistry.
 Double bond geometry as shown.



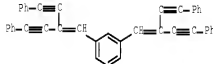
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
 REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2007:939644 CAPLUS Full-text
 DOCUMENT NUMBER: 147:385553
 TITLE: EDA Study of π -Conjugation in Tunable Bis(gem-diethynylethene) Fluorophores
 AUTHOR(S): Fernandez, Israel; Frenking, Gernot
 CORPORATE SOURCE: Fachbereich Chemie, Phillips-Universitaet Marburg, Marburg, D-35043, Germany
 SOURCE: Journal of Organic Chemistry (2007), 72(19), 7367-7372
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The strength of π -conjugation in a family of bis(gem-diethynylethene) fluorophores is estimated within the d. functional theory framework using the energy decomposition anal. (EDA) method. The observed very good linear correlations between the calculated π -conjugation and the exptl. values for the UV absorption and fluorescence emission for this series of compds. suggest that the values given by the EDA are useful for the interpretation and prediction of photochem. properties of the mols. The calculated data predict that adequate modifications in the core moiety of the mol. such as π -donor substituents in the aromatic ring or in the periphery of the bis-anadyne unit like π -acceptor groups placed in the para position of the aryl substituent increase the total π -conjugation in the systems and thus provoke significant

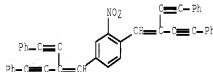
changes in both the absorption and emission spectra leading to large Stokes shifts. The effect of such substituents is quant. predicted by the EDA data.
 IT 360345-89-5 610283-06-2 610283-08-4
 610283-09-5 610283-10-6 610283-12-5
 950584-34-6
 RI: PRP (Properties)
 (experiment and calcul.; EDA study of π -conjugation in tunable bis(gem-diethynylethene) fluorophores)
 RN 360549-89-5 CAPLUS
 CN Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



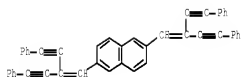
RN 610283-06-2 CAPLUS
 CN Benzene, 1,3-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



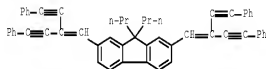
RN 610283-08-4 CAPLUS
 CN Benzene, 2-nitro-1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



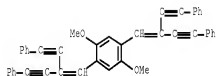
RN 610283-09-5 CAPLUS
 CN Naphthalene, 2,6-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



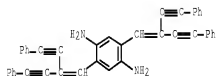
RN 610283-10-8 CAPLUS
CN 9H-Fluorene, 2,7-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-9,9-dipropyl- (CA INDEX NAME)



RN 610283-12-0 CAPLUS
CN Benzene, 1,4-dimethoxy-2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 950584-34-6 CAPLUS
CN 1,4-Benzenediamine, 2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



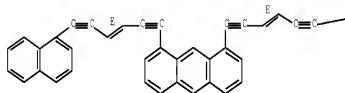
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STW
ACCESSION NUMBER: 2007:46877 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 148:284829
TITLE: Synthesis of smallest unit model of graphite

intercalation compound and its possibility
AUTHOR(S): Ogoshi, Sensuke
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Osaka University, Japan
SOURCE: Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku (2006) 01.03.07/1-01.03.07/3
CODEN: AGSHEN; ISSN: 0919-9179
PUBLISHER: Asahi Garasu Taikan
DOCUMENT TYPE: Journal; (computer optical disk)
LANGUAGE: Japanese
OTHER SOURCE(S): CASREACT 148:284829
AB Graphite is perhaps the simplest layered structure. Many substances can be intercalated between layers of graphite. Upon intercalation, the graphite layers moved apart somewhat due to the intercalated atom. However, the layers still keep parallel each other which would be the key for the formation of intercalation compds. Thus, compds. having two aromatic rings, which can change the distance between the rings and keep parallel to each other, were designed and synthesized. The target compound was 1,8-bis[(E)-3-hexene-1,5-diynyl]anthracene.
IT 1007602-95-02
RL: SPM (Synthetic preparation); PREP (Preparation)
(preparation of bis[(naphthalenyl)hexenediynyl]anthracene (smallest unit model for graphite intercalation compound))
RN 1007602-95-0 CAPLUS
CN Anthracene, 1,8-bis[(E)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



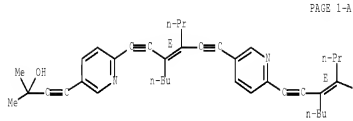
L10 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STW
ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 143:306181
TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki
PATENT ASSIGNER(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 82 pp.
COGEN: PIIKX2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

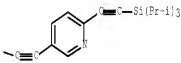
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-093950	20050308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
EW:	EW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AE, BY, EG, KG, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GW, GQ, GM, ML, MR, NE, SN, TD, TG			
US 20070176164	A1	20070802	US 2007-391950	20070307
PRIORITY APPL. INFO.:			JP 2004-65446	A 20040309
			WO 2005-093950	W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 143:306181

GI



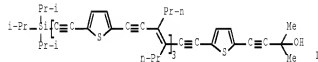
PAGE 1-A



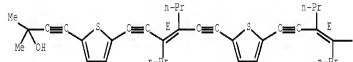
PAGE 1-B

RN 740810-68-8 CAPLUS
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

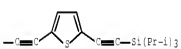
Double bond geometry as shown.



PAGE 1-A



PAGE 1-B



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-65-54 740810-68-8P 864683-97-6P
864684-52-5P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-(tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-methyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 864683-97-6 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-[5-ethynyl-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

*C#Cc1cc2c(c1)sc(C#CC3=CC(=C(C=C3)C(F)(F)F)C(F)(F)F)c2CC(C)(O)C(=O)c1cc(C)s1

Double bond geometry as shown.

CC(C)(O)C#Cc1ccc(C#C)nc1

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IT 740101-64-59 740101-69-39 865654-06-09
464644-01-19 865684-21-39 865684-22-49
740464-21-19 865684-26-14 865684-27-39
864684-28-09 865684-29-19 865684-30-09

RL: DEV (Device component use); INF (Industrial manufacture); SPN
(Synthetic preparation); TEM (Technical or engineered material use); PREP
(Preparation); USES (Uses)

[preparation of M-conjugated aromatic ring-containing acetylene derivs. as
organic
[electroluminescent devices)

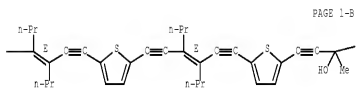
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Double bond geometry as shown.

$$(i\text{-Pr})_3\text{Si}-\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C}-\text{C}(\text{n-Pr})=\text{C}(\text{n-Pr})-\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C}-\text{Si}(i\text{-Pr})_3$$
CC(C)(C)C#CC1=CC=C(C=C1)C#CC(=C)C(=C)C#CC2=CC=C(C=C2)C#CC(=C)C(=C)C#CC3=CC=C(C=C3)C#CC(C)(C)C

Couple bond geometry as shown.

[Si]()*(C#Cc1ccsc1C#CC=C(C)C(=O)C#Cc2ccsc2C#C*)



PAGE 1-B

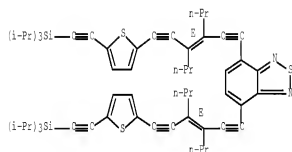


PAGE 1-C

RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

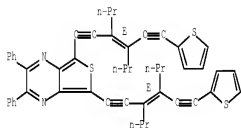
Double bond geometry as shown.



RN 864684-09-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

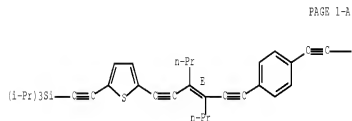
Double bond geometry as shown.



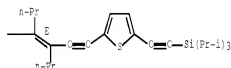
RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



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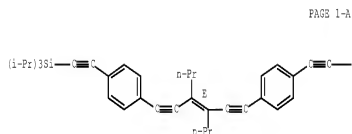


PAGE 1-B

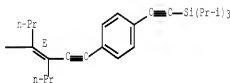
RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

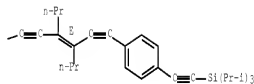


PAGE 1-B

RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

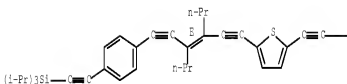


PAGE 1-B

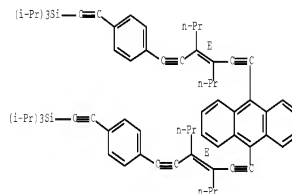
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

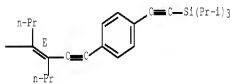
Double bond geometry as shown.



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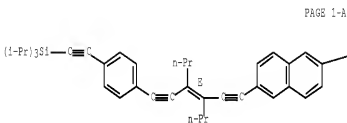
PAGE 1-B



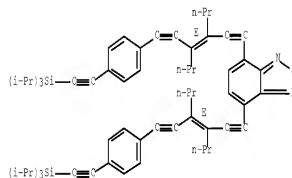
RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A



RN 864684-29-7 CAPLUS

PAGE 1-B

C=C(C)C#Cc1ccc(cc1)C#CC[Si]()
$$[(^t\text{-Pr})_3\text{Si}-\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C}-\text{C}(\text{n-Pr})=\text{C}(\text{n-Pr})-\text{C}\equiv\text{C}-\text{N} \begin{matrix} \diagup \\ \text{R} \\ \diagdown \end{matrix} \text{N}-\text{C}\equiv\text{C}]_n$$
*C=C(C)C#Cc1ccc(cc1)C#CSi(C)(C)C

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 of 22 CAPLUS COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 2005:354187 CAPLUS Full-text
DOCUMENT NUMBER: 143:333
TITLE: Cytotoxicities, cell cycle and caspase evaluations of
1,6-diaryl-3(2)-hexen-1,5-diyne,
2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their
derivatives

SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575

PUBLISHER: Elsevier Ltd.

LANGUAGE:

GT

64

Nc1ccccc1C#CC=CC#Cc2ccsc2

I

II

AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated

analogs were from <0.01 to 96.6 μ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10⁻⁷M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(2)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 852619-13-7P

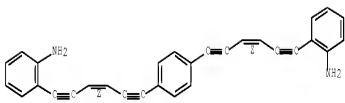
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); B10L (Biological study); PREP (Preparation)

(cytotoxicities, cell cycle and caspase evaluations of
1,6-diaryl-3(2)-hexen-1,5-diynes,
2-(6-aryl-3(2)-hexen-1,5-diynyl)anilines and their derivs.)

RN 852619-13-7 CAPLUS

CN Benzenamine, 2,2'-(1,4-phenylene)-di-(3Z)-3-hexene-1,5-diyn-6,1-diyl]bis-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS
RECORD (15 CITINGS)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2005:34387 CAPLUS Full-text

DOCUMENT NUMBER: 142:135171

TITLE: Liquid crystalline compound having perfluoroalkyl side
chains, liquid crystal composition containing these
compounds and their polymers

INVENTOR(S): Sasada, Yasuyuki; Yanai, Motoki

PATENT ASSIGNER(S): Chisso Petrochemical Corporation, Japan; Chisso
Corporation

SOURCE: U.S. Pat. Appl. Publ., 56 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

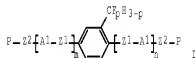
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050007541	A1	20050113	US 2004-873280	20040623
US 7070839	B2	20106704		

JP 2005035985 A 20050210 JP 2004-183449 20040622
PRIORITY APPLN. INFO.: JP 2003-177672 A 20030623
OTHER SOURCE(S): MARPAT 142:135171
GI



AB Liquid crystalline compds. I [P = CX22:CKXCO2, Q1, CKX2:CKXO, p-CKX2:CKXCO2R4, or Q2; A1 = 1,4-cyclohexenylene, 1,4-phenylene, naphthalene-2,6-diyl, tetrahydronaphthalene-2,6-diyl, fluorene-2,7-diyl, or bicyclo[2.2.2]octane-1,4-diyl, where any CH2 of these rings is optionally replaced by O, any CH is optionally replaced by N, and any H is optionally replaced by halo, C1-5 alkyl, or halogenated alkyl; Z1 = single bond, CH2CH2, CF2CF2, (CH2)4, CH2O, OCH2, CO2, OCO, CH:CH, CF4CF, C.tpbond.C, C.tpbond.CO2, OCO.C.tpbond.C, CH:CHCO2, OCOCH:CH, CH:CHCO2, OCOCH2CH2, C.tpbond.CCH:CH, CH:CH.C.tpbond.C, OCF2, or CF2; Z2 = single bond or C1-20 alkylene, where any CH2 is optionally replaced by O, S, CO2, or OCO; X1 = H, halo, CF3 or C1-5 alkyl, X2 = H, halo, or C1-5 alkyl; m, n = 0-2; m + n ≤ 4; p = 2 or 3; q = 0 or 1; when Z1 is C.tpbond.C, P = Q1, CKX2:CKXO, p-CKX2:CKXCO2R4] are prepared The invention further provides for polymerization of a composition containing 2l of I to give a film, an optical anisotropic material, a 1/4 or 1/2 wavelength functional plate, an optical compensation element, an optical element or a liquid crystal display element. A typical liquid crystalline compound (II) was manufactured by esterification of 2-(trifluoromethyl)-1,4-dihydroxybenzene with 4-(6-(acryloyloxy)hexyloxy)benzoic acid in THF in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide overnight. A typical liquid crystalline polymer was manufactured by photopolymerization of 80 parts II in a mixture containing 4-(trans-4-propylcyclohexyl)cyanobenzene 5, 4-(trans-4-pentylcyclohexyl)cyanobenzene 5, 4-(trans-4-heptylcyclohexyl)cyanobenzene 5, and 4'-(trans-4-heptylcyclohexyl)-4-cyano-1,1'-biphenyl 5 parts in the presence of Irgacure 907 as a film on a polyimide alignment film attached to a glass substrate.

IT 1056056-84-8

RI: PRPH (Prophetic)

(Liquid crystalline compound having perfluoroalkyl side chains, liquid
crystal composition containing these compounds and their polymers)

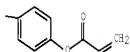
RN 1056056-84-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



PAGE 1-A



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2004:566840 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:261152

TITLE: π -Conjugated Dendrimers Based on Bis(enediynyl)benzene Units

AUTHOR(S): Hwang, Gil Tae; Kim, Byeang Hyeon

CORPORATE SOURCE: National Research Laboratory, Department of Chemistry,
Division of Molecular and Life Sciences, Pohang
University of Science and Technology, Pohang, 790-784,
S. Korea

SOURCE: Organic Letters (2004), 6(16), 2663-2672

COCODE: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have synthesized a new family of π -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The compds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.

IT 754233-15-SP 754233-16-AP 754233-17-SR

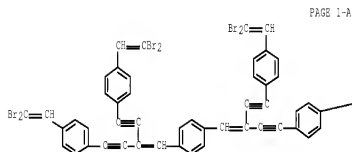
754233-14-SP

RL: RCT (Reactant); SPN (Synthetic preparation); PRDP (Preparation); RACT (Reactant or reagent)

(convergent and divergent synthesis of π -conjugated dendrimers based on bis(enediynyl)benzene units)

RN 754233-15-3 CAPLUS

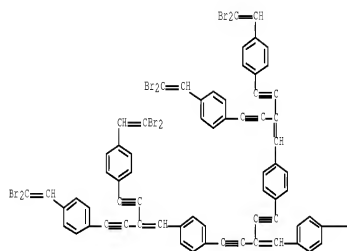
CN Benzene, 1,4-bis[4-(4-(2,2-dibromoethynyl)phenyl)-2-[[4-(2,2-dibromoethynyl)phenyl]ethynyl]-1-buten-3-ynyl]- (3CI) (CA INDEX NAME)



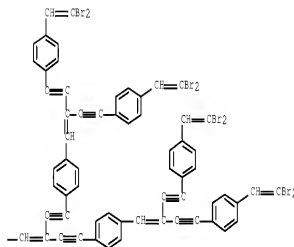
PAGE 1-A

RN 754233-16-4 CAPLUS

CN Benzene, 1,4-bis[4-(4-(4-(2,2-dibromoethynyl)phenyl)-2-[[4-(2,2-dibromoethynyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-(4-(4-(2,2-dibromoethynyl)phenyl)-2-[[4-(2,2-dibromoethynyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



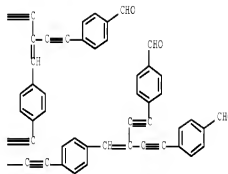
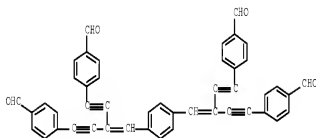
PAGE 1-A



PAGE 1-B

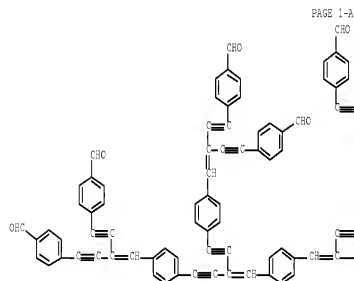
RN 754233-17-5 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-(4-(4-formylphenyl)-2-((4-formylphenyl)ethynyl)-1-buten-3-ynyl]phenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)



RN 754233-18-6 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-(4-(4-(4-formylphenyl)-2-((4-formylphenyl)ethynyl)-1-buten-3-ynyl]phenyl)-2-[[4-(4-(4-formylphenyl)ethynyl)-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yn-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)



CS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

110 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:430115 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

AUTHOR(S): Makano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji;

Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

SOURCE: Organic Letters (2004), 6(14), 2373-2376

CODEN: ORLEF7; ISSN: 1523-7060

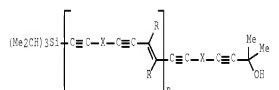
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

GI



AB Synthesis and fluorescence properties of π -conjugated compds. 1 ($n = 1 - 3$; $X = 1,4$ -phenylene, 2,5-pyridine, 2,5-thiophene; $R = n$ -Pr, n -Bu) having

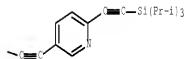
alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

IT 740810-62-2P 740810-65-5P 740810-68-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

PAGE 1-B



RN 740810-62-2 CAPLUS

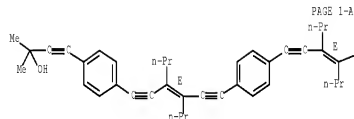
CN 3-Butyn-2-ol, 2-methyl-4-[[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

RN 740810-68-8 CAPLUS

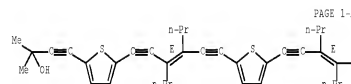
CN 3-Butyn-2-ol, 2-methyl-4-[[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.

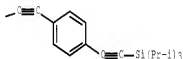


PAGE 1-A

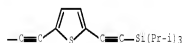


PAGE 1-A

PAGE 1-B



PAGE 1-B



RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

IT 740810-65-5P 740810-66-6P 740810-69-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

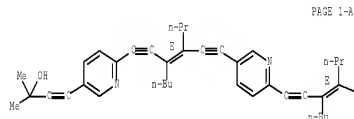
(preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-63-3 CAPLUS

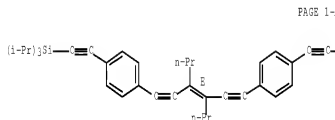
CN 3-Butyn-2-ol, 2-methyl-4-[[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

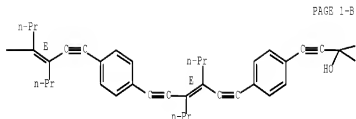
Double bond geometry as shown.



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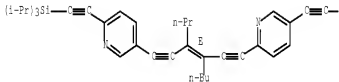
PAGE 1-C



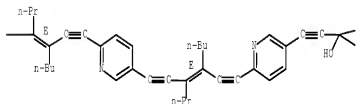
RN 740810-66-6 CAPLUS
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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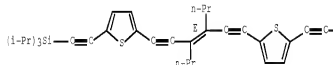
PAGE 1-C



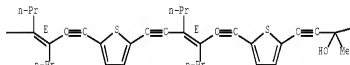
RN 740810-69-9 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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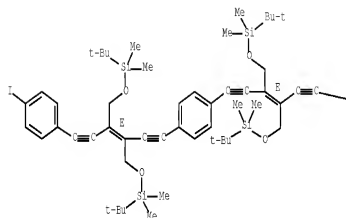
OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

110 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:328526 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 141:54000
TITLE: Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylacetacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions
AUTHOR(S): Utesch, Wils F.; Diederich, Francois; Boudon, Corinne; Glsselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg,
 HCI, Zurich, CH-8093, Switz.
 SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718
 CODEN: HCACNV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:54000

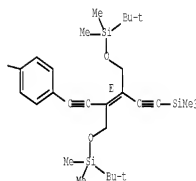
PAGE 1-A

AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodophenyl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-1[CGH4C.tpbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tpbond.C]nSiMe3 (I, n = 2-4) a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I (n = 1-4) shift bathochromically with increasing oligomeric length, from λ_{max} 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π -Electron conjugation in these oligomers is less efficient than in



PAGE 1-B

Me3Si[CGH4C.tpbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tpbond.C] nSiMe3 (II) due to poor transmittance of π -electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield $\Phi_F = 0.69$ measured for I (n = 3). Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.



IT 554459-63-1P 554459-64-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (solid-phase synthesis of oligo(triacetylene)s and
 oligo(phenylene triacetylene)s by Sonogashira and Cadiot-Chodkiewicz
 cross-coupling reactions)

RN 554459-63-1 CAPLUS

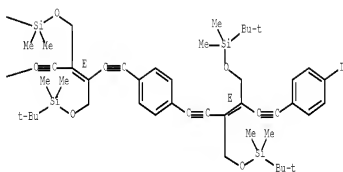
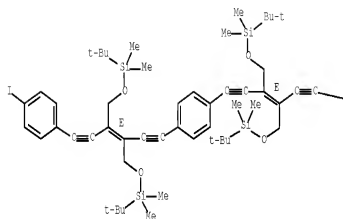
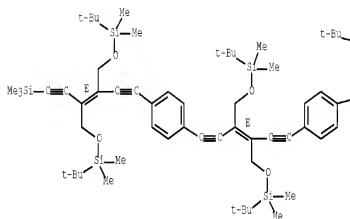
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-([4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl)-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-([4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl)-7-([4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl)-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.



IT 704916-29-06

RL: SPM (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of oligo(triacetylene)s and
oligo(phenylenetriacetylene)s by Sonogashira and Cadot-Chodkiewicz
cross-coupling reactions)

RN 704916-29-0 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-
ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,3,10,10,11,11-octamethyl-,
(6E,6'E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

CS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

110 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2003:827385 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:59755

TITLE: Synthesis and reactivity of dinuclear rhodium
complexes with Rh:C:CHR and Rh:C:C:CHR' units as
building blocks

AUTHOR(S): Callejas-Gaspar, Berta; Laubender, Matthias; Werner,
Helmut

CORPORATE SOURCE: Institut fuer Anorganische Chemie der Universitaet
Wuerzburg, Wuerzburg, D-97074, Germany

SOURCE: Journal of Organometallic Chemistry (2003), 684(1-2),
144-152

CODEN: JORCAL; ISSN: 0022-328X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:59755

AB The reaction of [Rh(k2-C2S(O)CF3)(Pip3)2] (1) with ethynylferrocene in the
presence of KF affords the substituted vinylidene complex trans-

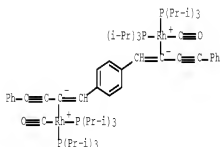
[RhF(C6H4(C5H4)Fe(C5H5))(P(Pr)3)2] (2) which upon treatment with the butadiene derivative Ph3SnC.tlpbond.C-C.tlpbond.C5H9 produces the chair-like compound trans-[μ-(C.tlpbond.C-C.tlpbond.C)(Rh(C6H4(C5H4)Fe(C5H5))(P(Pr)3)2)2] (7). The triflate complex 1 reacts with 1,4-C6H4(C.tlpbond.CH)2 to give the dinuclear compound trans-[μ-1,4-C6H4(CH(C)2)(Rh(η1-OS(0)2CF3)(P(Pr)3)2)2] (3) in which in the presence of KF undergoes a ligand exchange to give the corresponding difluoro derivative trans-[μ-1,4-C6H4(CH(C)2)(RhF(P(Pr)3)2)2] (4). From 4 and 8C.tlpbond.C5H9Ph3 (R = CH3, C6H5) the complexes trans-[μ-1,4-C6H4(CH(C)2)(Rh(C.tlpbond.CR)(P(Pr)3)2)2] (5) and (6), in which a C6H4 unit bridges two alkynyl(vinylidene)rhodium(I) fragments, are obtained. Both 6 and 7 react with CO by migratory insertion of the vinylidene units into the alkynyl-metal bonds to afford the dinuclear complexes trans-[μ-(2,2'-C(C)(CH(C5H4)Fe(C5H5)))(Rh(CO)(P(Pr)3)2)2] (8) and trans-[μ-(2,2'-C(C.tlpbond.CPh)(CH(C6H4CH(C)C(C.tlpbond.CPh)))(Rh(CO)(P(Pr)3)2)2] (9), in which an unusual C8 or C4(C6H4)C4 chain bridges the two rhodium centers. The reactions of [RhCl(P(Pr)3)2]2 (10) with the functionalized diynes 1,1',4,4'-C6H4(OH)2(C.tlpbond.CH)2 and 1,4-C6H4(C(Ph)(OH)C.tlpbond.CH)2 lead, via the corresponding diyne-metal species (11) and (12) as intermediates, to the formation of the bis(vinylidene) complexes (13) and (14), the latter of which reacts with acidic Al2O3 by elimination of water to give the novel phenylene-bridged bis(allylidenetandium) compound [μ-1,4-C6H4(CH(C)C(C)2)(RuCl(P(Pr)3)2)2] (15) in 80% yield.

IT 639078-94-39

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactivity of dinuclear rhodium carbene and alkynyl complexes)

RN 639078-96-9 CAPLUS

CN Rhodium, dicarbonyl[μ-[1,4-phenylenebis(12)-1-(phenylethynyl)-2,1-etheradiyl]]tetrakis[tris(1-methylethynyl)phosphine]di-, stereoisomer (9CI)
(CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2003:648967 CAPLUS Full-text

DOCUMENT NUMBER: 139:308866

TITLE: Synthesis and photophysical studies of bis-enediynes as tunable fluorophores

AUTHOR(S): Hwang, Gil Tae; Son, Hyung Su; Ku, Ja Kang; Kim, Byeang Hyeon

CORPORATE SOURCE: National Research Laboratory, Center for Integrated Molecular Systems, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Journal of the American Chemical Society (2003), 125(37), 11241-11248
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:308866

AB We have synthesized a family of bis-enediynes by two complementary Pd/Cu-catalyzed Sonogashira cross-coupling methods. One is a modified Sonogashira reaction between a TMS-protected tetraalkyne and various aromatic bromides to afford bis-enediynes bearing different peripheral aryl units. The other, the reaction of bifunctional 1,1-dibromo-1-alkenes with phenylacetylene, afforded a series of bis-enediynes bearing various core aryl groups. These chemical modifications to the core and periphery of bis-enediynes induce dramatic changes in absorption and emission spectra. Bis-enediynes with peripheral aryl groups show a large Stokes shift of about 50-110 nm when compared to the less-conjugated TMS-protected bis-enediynes. Absorptions and emissions of other bis-enediynes were red-shifted relative to those of (4-phenyl-2-phenylethynyl)-1-buten-3-ynylbenzene. Substantial increases in fluorescence quantum yields are observed as a result of extending the π-conjugation. The emission wavelength of the bis-enediynes was tailored from indigo blue to reddish-orange, suggesting that the color of emission can be tunable by modification of the core and/or peripheral units.

IT 360549-89-94 360549-90-2P 360549-91-3P

360549-92-4P 360549-93-2P 360549-94-5P

360549-95-7P 360549-96-0P 360549-97-5P

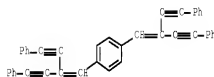
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360549-11-3P 360549-12-4P 360549-13-1P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USDS (Uses)
(dye; preparation and photophysics properties of bis-enediynes as tunable fluorophores)

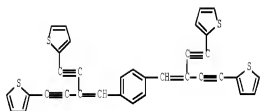
RN 360549-89-9 CAPLUS

CN Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

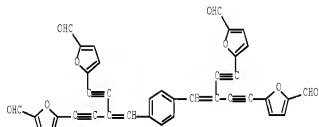


RN 360549-90-2 CAPLUS

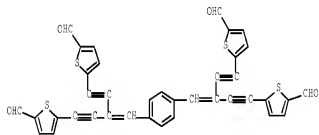
CN Thienophene, 2,2'-[1,4-phenylenebis[3-(2-thienylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



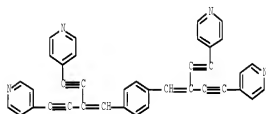
RN 360549-91-3 CAPLUS
CN 2-Furancarboxaldehyde, 5,5'-(1,4-phenylenebis[3-((5-formyl-2-furanyl)ethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



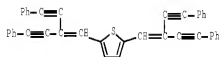
RN 360549-92-4 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5,5'-(1,4-phenylenebis[3-((5-formyl-2-thienyl)ethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



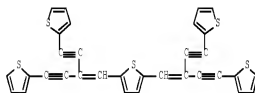
RN 360549-93-5 CAPLUS
CN Pyridine, 4,4'-(1,4-phenylenebis[3-(4-pyridinylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



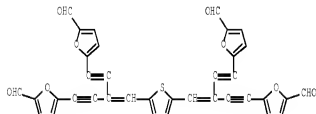
RN 360549-94-6 CAPLUS
CN Thiophene, 2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



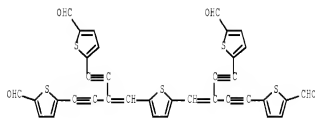
RN 360549-95-7 CAPLUS
CN Thiophene, 2,5-bis[4-(2-thienyl)-2-(2-thienylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 360549-96-8 CAPLUS
CN 2-Furancarboxaldehyde, 5,5'-(2,5-thiophenediylbis[3-((5-formyl-2-furanyl)ethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

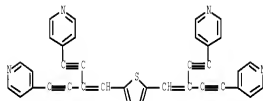


RN 360549-97-9 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5,5'-(2,5-thiophenediylbis[3-((5-formyl-2-thienyl)ethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



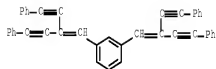
RN 360549-98-0 CAPLUS

CN Pyridine, 4,4'-[2,5-thiophenediylbis(3-(4-pyridinylethynyl))-3-buten-1-yne-4,1-diyl]bis- (9CI) (CA INDEX NAME)



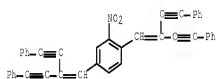
RN 610283-06-2 CAPLUS

CN Benzene, 1,3-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



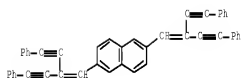
RN 610283-08-4 CAPLUS

CN Benzene, 2-nitro-1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



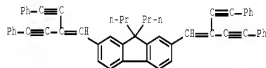
RN 610283-09-5 CAPLUS

CN Naphthalene, 2,6-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



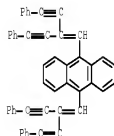
RN 610283-10-8 CAPLUS

CN 9H-Fluorene, 2,7-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-9,9-dipropyl- (CA INDEX NAME)



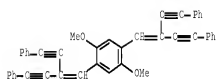
RN 610283-11-9 CAPLUS

CN Anthracene, 9,10-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



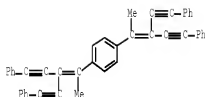
RN 610283-12-0 CAPLUS

CN Benzene, 1,4-dimethoxy-2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 610283-13-1 CAPLUS

CN Benzene, 1,4-bis[1-methyl-4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 44 THERE ARE 44 CAPLUS RECORDS THAT CITE THIS
RECORD (44 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:424696 CAPLUS Full-text
DOCUMENT NUMBER: 139:150012
TITLE: Synthesis of Highly Fluorescent Y-Enyne Dendrimers
with Four and Six Arms
AUTHOR(S): Kaafarani, Bilal R.; Wex, Brigitte; Wang, Fei;
Catanescu, Otilia; Chien, L. C.; Neckers, Douglas C.
CORPORATE SOURCE: Center for Photochemical Sciences, Bowling Green State
University, Bowling Green, OH, 43403, USA
SOURCE: Journal of Organic Chemistry (2003), 68(13), 5377-5380
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

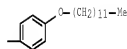
AB A first generation of dendrimeric Y-enynes with extended flexible chains was
synthesized using Sonogashira coupling. Dendrimers 9 and 10 are highly
fluorescent in the solid state and in solution

IT 569670-22-06 569670-23-1P

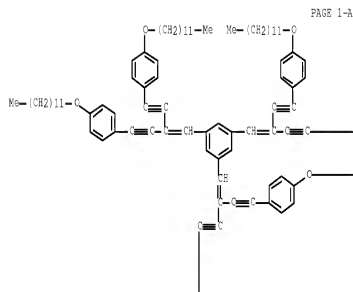
RL: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of highly fluorescent Y-enyne dendrimers with four and six
arms)

RN 569670-22-0 CAPLUS

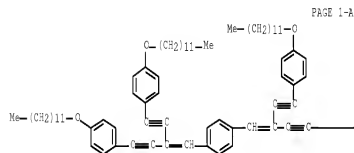
CN Benzene, 1,4-bis[4-[4-(dodecyloxy)phenyl]-2-[[4-(
dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (3CI) (CA INDEX NAME)



RN 569670-23-1 CAPLUS
CN Benzene, 1,3,5-tris[4-[4-(dodecyloxy)phenyl]-2-[[4-(
dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (3CI) (CA INDEX NAME)

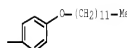


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PAGE 1-B

—(CH₂)₁₁—Me



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 2003:234291 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:85055

TITLE: Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadot-Chodkiewicz-type cross-coupling reactions

AUTHOR(S): Utesch, Nils F.; Diederich, Francois

CORPORATE SOURCE: Laboratorium für Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.

SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239

CODEN: OBCKAY, ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:85055

AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., 1[4-CH4C.tplbond.CCR:CRG.tplbond.C]nSiMe3 (R = CH2OSiBuMe2, n = 1, 2, 3, 4) members of a new class of linearly π -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

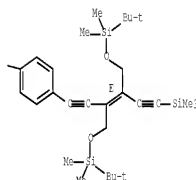
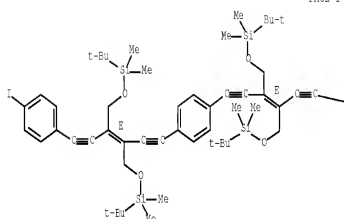
IT 554459-62-19 554459-64-2P

EL: PREP (Properties); SYN (Synthetic preparation); PREP (Preparation) (electronic absorption and emission, UV/VIS spectra); poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)

RN 554459-63-1 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-([4-((3E)-6-[4-((3E)-3,4-bis([[(1,1-dimethylethyl]dimethylsilyl)oxy]methyl)-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl)-3,4-bis([[(1,1-dimethylethyl]dimethylsilyl)oxy]methyl)-3-hexene-1,5-diynyl]phenyl)ethynyl)-2,2,3,3,10,10,11,11-octamethyl-7-([trimethylsilyl]ethynyl)-, (6E)- (9CI) (CA INDEX NAME)

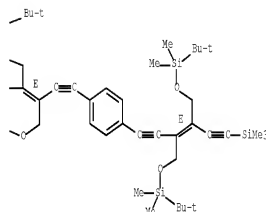
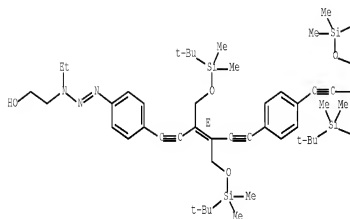
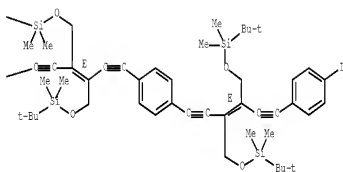
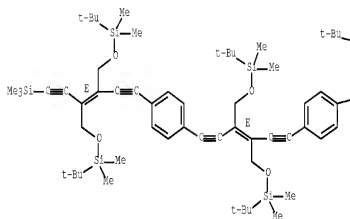
Double bond geometry as shown.



RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-([4-((3E)-6-[4-((3E)-3,4-bis([[(1,1-dimethylethyl]dimethylsilyl)oxy]methyl)-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl)-3,4-bis([[(1,1-dimethylethyl]dimethylsilyl)oxy]methyl)-3-hexene-1,5-diynyl]phenyl)ethynyl)-7-([4-((3E)-3,4-bis([[(1,1-dimethylethyl]dimethylsilyl)oxy]methyl)-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl)ethynyl)-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 554459-70-06, Merrifield resin-supported
 554459-70-06, Merrifield resin-supported
 RI: RCT (Reactant); SPN (Synthetic preparation); PRDP (Preparation); RACT
 (Reactant or reagent)
 (preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed
 cross-coupling reactions of supported poly(triacetylene)-derived
 oligomers)
 RN 554459-72-2 CAPLUS
 CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-
 dimethylethyl]dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-
 diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
 hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
 hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
 hexene-1,5-diyn-1-yl]phenyl]-2-triazen-1-yl]- (CA INDEX NAME)

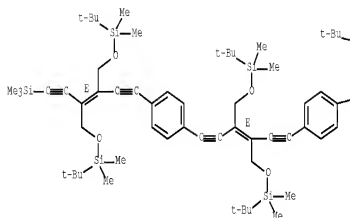
RN 554459-73-3 CAPLUS
 CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-
 dimethylethyl]dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-
 diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
 hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
 hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-
 hexene-1,5-diyn-1-yl]phenyl]-2-triazen-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

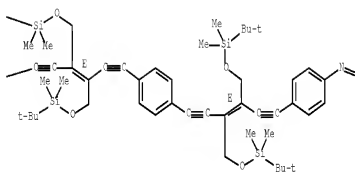
Double bond geometry as described by E or Z.

DOCUMENT NUMBER: 136:69640
 TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units
 AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Baley, Michael M.
 CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA
 SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490
 CODEN: EJOCYH; ISSN: 1434-193X
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:69640
 GI

PAGE 1-A



PAGE 1-B

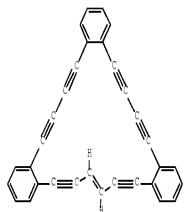


PAGE 1-C



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)
 REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

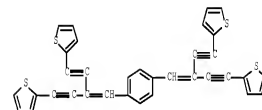
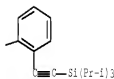
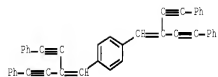
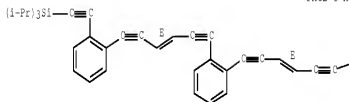
L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2009 ACS on STM
 ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzannulation.

IT 367064-38-4P
 RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)
 RN 383494-38-4 CAPLUS
 CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diene-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2001:519766 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:243732

TITLE: Novel fluorophores: efficient synthesis and photophysical study

AUTHOR(S): Hwang, Gil Tae; Son, Hyung Su; Ku, Ja Kang; Kim, Byeang Hyeon

CORPORATE SOURCE: Center for Integrated Molecular Systems Department of Chemistry Division of Molecular Life Science, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Organic Letters (2001), 3(16), 2469-2471

COGEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:243732

AB We have synthesized novel tetraacetylenic fluorophores by using Sonogashira reactions of 1,4-bis(dibromovinyl)benzene and 2,5-bis(dibromovinyl)thiophene with various aromatic bromides. The emission maxima of these fluorophores vary from the indigo blue to the reddish-orange region, depending on the structures of the aromatic nuclei and peripheral moieties.

IT 360549-49-5P 360549-50-2P 360549-81-2P
360549-52-4H 360549-53-5N 360549-94-6P
360549-75-7P 360549-96-8C 360549-97-3H
360549-98-0P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(fluorescent dye; preparation and spectra of tetraacetylenic fluorophores)

RN 360549-89-9 CAPLUS

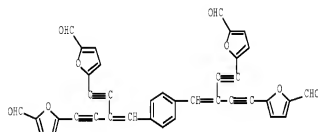
CN Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA

RN 360549-90-2 CAPLUS

CN Thiophene, 2,2'-[1,4-phenylenebis[3-(2-thienylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

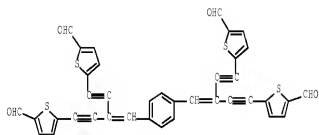
RN 360549-91-3 CAPLUS

CN 2-Furancarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



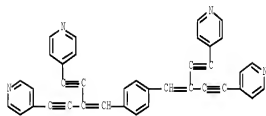
RN 360549-92-4 CAPLUS

CN 2-Thiophenecarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



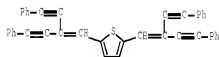
RN 360549-93-5 CAPLUS

CN Pyridine, 4,4'-[1,4-phenylenebis[3-(4-pyridinylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



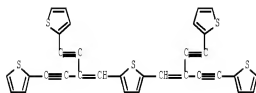
RN 360549-94-6 CAPLUS

CN Thiophene, 2,5-bis[4-(2-phenylethynyl)-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



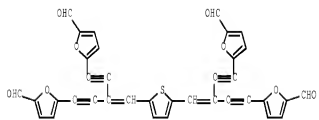
RN 360549-95-7 CAPLUS

CN Thiophene, 2,5-bis[4-(2-thienyl)-2-(2-thienyl)ethynyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)



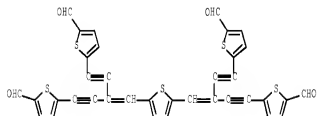
RN 360549-96-8 CAPLUS

CN 2-Furanocarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-furyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



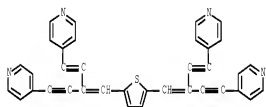
RN 360549-97-9 CAPLUS

CN 2-Thiophenecarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 360549-98-0 CAPLUS

CN Pyridine, 4,4'-[2,5-thiophenediylbis[3-(4-pyridinylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

110 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1996:29553 CAPLUS [Full-Text](#)

DOCUMENT NUMBER: 124:260436

ORIGINAL REFERENCE NO.: 124:48247a,48250a

TITLE: Synthesis and reactions of new ethynyl-substituted 1,6-methano[10]annulenes

AUTHOR(S): Bryant-Freidrich, Amanda; Weidlein, Richard
CORPORATE SOURCE: Pharm.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-69120, Germany

SOURCE: Synthesis (1995), (12), 1506-10

PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:260436
GI



AB Stereospecific Pd(PPh₃)₄ catalyzed coupling of an acetylene to geminal dibromo-substituted alkenes yielded enynes, which upon dehydrohalogenation formed butadiynyl substituted 1,6-methano[10]annulenes 1 [R = (C.tplbond.C)2R3; R1 = R2 = H, R3 = Ph, CMe3; R1 = H, R = R2 = (C.tplbond.C)2R3; R = R1 = (C.tplbond.C)2R3, R2 = H].

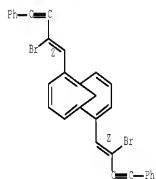
IT 175430-09-8 175430-11-2
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of ethynyl-substituted methanoannulenes)

RN 175430-09-8 CAPLUS

CN Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene, 2,7-bis(2-bromo-4-phenyl-1-buten-3-ynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)

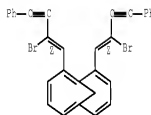
Double bond geometry as shown.



RN 175430-11-2 CAPLUS

CN Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene, 2,10-bis(2-bromo-4-phenyl-1-buten-3-ynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



110 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:192448 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 120:192448

ORIGINAL REFERENCE NO.: 120:34087a,34090a

TITLE: Synthesis of a series of conjugated enyne polythiophenes

AUTHOR(S): Kane, James J.; Gao, Feng; Reinhardt, Bruce A.; Dvers, Robert C.

CORPORATE SOURCE: Chem. Dep., Wright State Univ., Dayton, OH, 45435-0001, USA

SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1992), 33(1), 1064-5
CODEN: ACPPAY; ISSN: 0032-3934

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title polymers were prepared via polymerization of 3,4-didecyloxy-2,5-bis-(β-bromoethenyl)thiophene and aromatic diethynyl compds. Thermal and viscosity of the resulting thiophene-containing polyacetylenes are discussed.

IT 153846-90-3

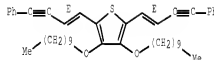
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and polymerization of, with aromatic diethynyl compds.)

RN 153846-90-3 CAPLUS

CN Thiophene, 3,4-bis(decyloxy)-2,5-bis(4-phenyl-1-buten-3-ynyl)-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

110 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:23114 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 100:23114

ORIGINAL REFERENCE NO.: 100:3653a,3656a

TITLE: Cis-Dynne aromatic and aromatic heterocyclic polymers

INVENTOR(S): Reinhart, Bruce

PATENT ASSIGNER(S): United States Dept. of the Air Force, USA

SOURCE: U. S. Pat. Appl., 4 pp. Avail. NTIS Order No.

PAT-APPL-6-399 661.
 CODEN: XAXXAV
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 399661	A0	19830304	US 1982-399661	19820719
US 4417039	A	19831122		

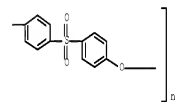
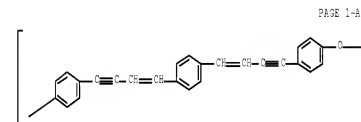
PRIORITY APPL. INFO.: US 1982-399661 19820719

AB Aromatic and aromatic heterocyclic enyne polymers having relatively low glass temps. for fabrication are prepared by treating 1,4-bis(cis- β -bromovinyl)benzene (I) [88248-70-8] with a diacetylenic compound. The polymers exhibit high glass temps. and low solvent susceptibilities after heat treatment. Thus, a suspension of 40 g p-phenylenediacrylic acid [16323-43-6] in 300 g Br was stirred for 3 h to give β,β' -p-phenylenebis(α,β -dibromopropionic acid) (II) [88248-71-9]. A mixture of 21.5 g II and 20.0 g NaHCO₃ in 500 mL acetone was refluxed for 72 h to give I. A mixture of 0.5 g I and 0.7658 g 4,4'-bis(3-ethynylphenoxy)diphenyl sulfone [63770-82-1] was dissolved in a solution of 3 mL Et₃N and 3 mL N,N-dimethylacetamide (III). A mixture of 0.025 g CuI and 0.05 g (Ph₃P)₂PdCl₂ was added. The mixture was stirred at room temperature for 70 h. Addnl. 10 mL III was added to give a polymer having glass temperature 143°. The polymer [88249-72-3] treated at 250° for 6 h had glass temperature >375° and was insol. in solvents.

IT 88248-70-1P 88249-71-7P 88249-72-3P
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (manufacture of, with low glass temperature)

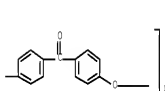
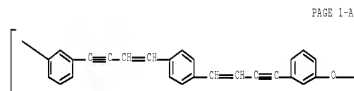
RN 88249-70-1 CAPLUS

CN Poly(oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,4-phenylene), (Z,Z)-(9CI) (CA INDEX NAME)



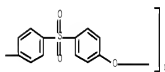
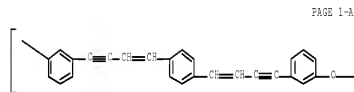
RN 88249-71-2 CAPLUS

CN Poly(oxy-1,4-phenylenecarbonyl-1,4-phenyleneoxy-1,3-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,3-phenylene), (Z,Z)-(9CI) (CA INDEX NAME)



RN 88249-72-3 CAPLUS

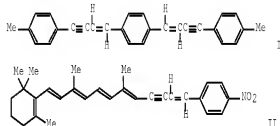
CN Poly(oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,3-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,3-phenylene), (Z,Z)-(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

110 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1981:175327 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 94:175327
 ORIGINAL REFERENCE NO.: 94:28659a,28662a
 TITLE: Reactions with phosphinealkynes. XXXIX. New methods for the preparation of 1-bromoacetylenes and aromatic and conjugated enynes
 AUTHOR(S): Bestmann, Hans Juergen; Frey, Herbert
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Erlangen-Muenberg, Erlangen, D-8520, Fed. Rep. Ger.
 SOURCE: Liebig's Annalen der Chemie (1990), (12), 2061-71
 CODEN: LACHEH; ISSN: 0170-2041
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 94:175327
 GI

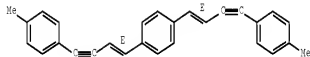


AB Some of RCH:CBR2 [R = optionally substituted Ph, naphthyl, 9-anthryl, 2-thienyl, alkyl, cycloalkyl, MeCH:OMe, MeCH:CH, MeCH:CHCH:CH, MeC:CHCH2CH:CH:CH, retinyl, 2-furyl, PhCH:CH, PhCH:OMe], prepared in 23-85% yields from RCHO, PPh3 and CBr4, were dehydrobrominated with (PhCH2)MgBr-OH- to give 35-80% RC:tpbond.CBR (R = optionally substituted Ph, naphthyl, 9-anthryl, alkyl, cycloalkyl), which were treated with Ph3P=MeBr- and R'CHO [R1 = 4-O2C6H4, 9-anthryl, 3,4-Cl2C6H3, 3,4,5-(MeO)3C6H2, piperonyl, nicotiny, 2-furyl, PhCH:CH] to give 20-70% RC:tpbond.CBR:CBRL. Addnl. obtained were 28% I and 35% II.

IT 77235-35-3P
 RL: SPW (Synthetic preparation); PREP (Preparation) (preparation of)

RN 77295-85-3 CAELUS
 CN Benzene, 1,4-bis[4-(4-methylphenyl)-1-buten-3-ynyl]-, (E,E)- (9CI) (CA INDEX NAME)

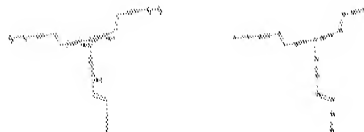
Double bond geometry as shown.



OS.CITING REF COUNT: 30 THERE ARE 30 CAPLUS RECORDS THAT CITE THIS RECORD (30 CITINGS)

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 17-18 18-19 19-20 26-27 27-28 28-29 29-30 30-31 31-32 32-33
 exact/norm bonds :
 4-5 5-6 11-12 12-13 12-26 18-19 19-20 31-32 32-33
 exact bonds :
 6-7 7-8 8-9 9-10 10-11 13-14 14-15 15-16 16-17 17-18 26-27 27-28 28-29
 29-30 30-31

G1:Cb,Cy,By

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Sl,Cb,Cy,By

Match level :
 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
 26:CLASS 27:CLASS
 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS

L11 STRUCTURE UPLOADED

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100.04 PROCESSED 11407 ITERATIONS 2 ANSWERS
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L12 2 SEA SSS FUL L11

=> file caplus

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L13 2 L12

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YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STM

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuzuki

PATENT ASSIGNOR(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

COENR: P1XX02

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

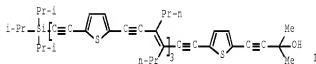
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 20050985176	A1	20050915	WO 2005-JP3950	20050909
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BW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SI, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, EG, GZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2007016164	A1	20070802	US 2007-591950	20070307
PRIORITY APPL. INFO.: JP 2004-65446 A 20040309				
			WO 2005-JP3950	W 20050909

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): HARPAT 143:306181

G1



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of

palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compo. are useful as electroluminescent devices.

IT 864684-30-00

RI: DEV (Device component use); IMF (Industrial manufacture); SPN

(Synthetic preparation); TEM (Technical or engineered material use); PREP

(Preparation); USES (Uses)

(preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic

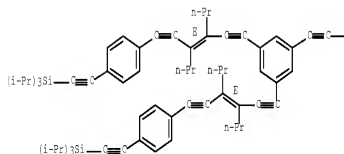
electroluminescent devices)

RN 864684-30-0 CAPLUS

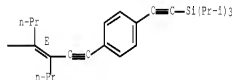
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STM

ACCESSION NUMBER: 2003:424686 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:150012

TITLE: Synthesis of Highly Fluorescent Y-Znyme Dendrimers with Four and Six Arms

AUTHOR(S): Maafarani, Bilal R.; Wax, Brigitte; Wang, Fei;

Catanescu, Otilia; Chien, L. C.; Neckers, Douglas C.

CORPORATE SOURCE: Center for Photochemical Sciences, Bowling Green State

University, Bowling Green, OH, 43403, USA

SOURCE: Journal of Organic Chemistry (2003), 68(13), 5377-5380

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A first generation of dendrimeric Y-enynes with extended flexible chains was synthesized using Sonogashira coupling. Dendrimers 9 and 10 are highly fluorescent in the solid state and in solution
 IT 569670-23-19
 RL: PREP (Properties); SPW (Synthetic preparation); PREP (Preparation)
 (synthesis of highly fluorescent Y-enyne dendrimers with four and six arms)
 RN 569670-23-1 CAPLUS
 CN Benzene, 1,3,5-tris[4-[4-(dodecyloxy)phenyl]-2-[[4-(dodecyloxy)phenyl]ethynyl]-1-butan-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 2-A



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)
 REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

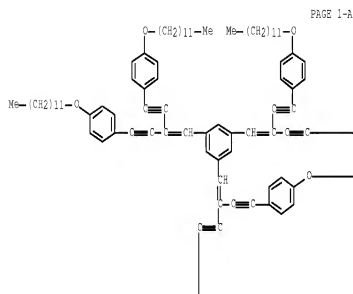
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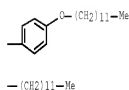
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PAGE 1-B



chain nodes :
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 chain bonds :
 4-5 5-6 6-7 6-10 7-8 7-11 8-9
 exact/norm bonds :
 6-10 7-11
 exact bonds :
 4-5 5-6 6-7 7-8 8-9

G1:Cb,Cy,By

G2:C,H,O,N,C1,Br,F,I

G3:C,H,Si,Cb,Cy,By

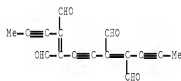
RN 937386-11-3 CAPLUS
CN 4,8-Dodecadiene-2,6,10-triyne (CA INDEX NAME)

CN 2,6-Octadien-4-ynediacarboxaldehyde, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-12-4 CAPLUS

CN 4,8,12-Hexadecatetriene-2,6,10,14-tetrayne (CA INDEX NAME)

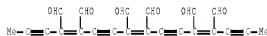
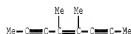


RN 937386-21-5 CAPLUS

CN 4,8,12-Hexadecatetriene-2,6,10,14-tetrayne-4,5,8,9,12,13-hexacarboxaldehyde (CA INDEX NAME)

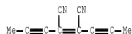
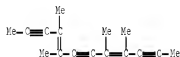
RN 937386-13-5 CAPLUS

CN 4-Octene-2,6-diyne, 4,5-dimethyl- (CA INDEX NAME)



RN 937386-14-6 CAPLUS

CN 4,8-Dodecadiene-2,6,10-triyne, 4,5,8,9-tetramethyl- (CA INDEX NAME)

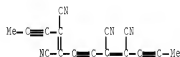
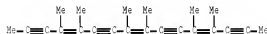


RN 937386-23-7 CAPLUS

CN 2,6-Octadien-4-ynetetracarboxitrile, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)

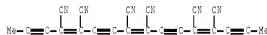
RN 937386-15-7 CAPLUS

CN 4,8,12-Hexadecatetriene-2,6,10,14-tetrayne, 4,5,8,9,12,13-hexamethyl- (CA INDEX NAME)



RN 937386-19-1 CAPLUS

CN 2-Butenedial, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-20-4 CAPLUS

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER: 20051004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 62 pp.

CODEN: PIXX22

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

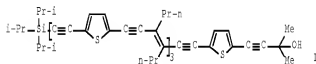
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005098176	A1	20050915	WO 2005-IP3950	20050308
W: AG, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EG, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SN, ST, TD, TH, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AG, AI, AT, BG, BR, CA, CH, CN, CO, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPL. INFO.: JP 2004-65446 A 20040309				
WO 2005-IP3950 W 20050308				

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN L5US DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI



AB This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-64-4P 740910-65-3P 740910-66-7P

740910-67-8P 864883-98-5P 864883-99-6P

864884-01-7P 864884-02-8P 864884-03-9P

864884-04-0P 864884-05-1P 864884-06-2P

864884-07-3P 864884-08-4P 864884-09-5P

864884-10-6P 864884-11-7P 864884-12-8P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

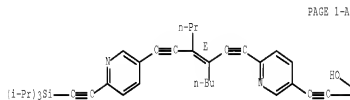
(intermediate; preparation of π -conjugated aromatic ring-containing acetylene

derivs. as organic electroluminescent devices)

RN 740910-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

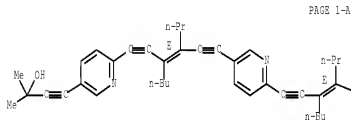


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RN 740810-65-5 CAPLUS

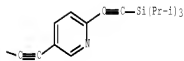
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

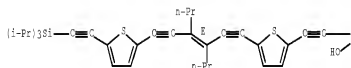
PAGE 1-B



RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



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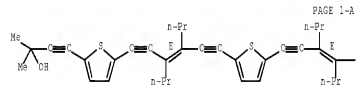


PAGE 1-B

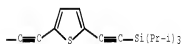
RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



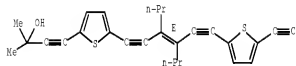
PAGE 1-B



RN 864683-96-5 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

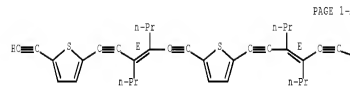
Double bond geometry as shown.



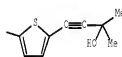
RN 864683-97-6 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-(5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



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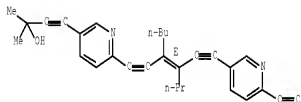


PAGE 1-B

RN 864684-01-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

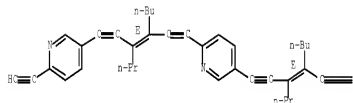


RN 864684-02-6 CAPLUS

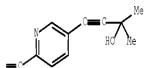
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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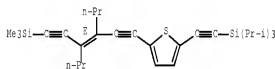
PAGE 1-B



RN 864684-04-8 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

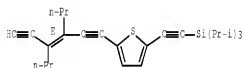
Double bond geometry as shown.



RN 864684-05-9 CAPLUS

CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

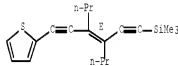
Double bond geometry as shown.



RN 864684-07-1 CAPLUS

CN Thiophene, 2-[(3E)-5-ethyl-3-propyl-4-[2-(trimethylsilyl)ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)

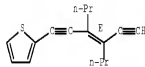
Double bond geometry as shown.



RN 864684-08-2 CAPLUS

CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

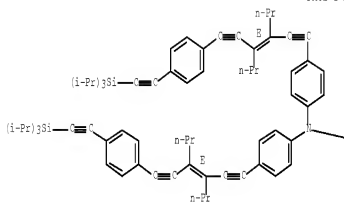


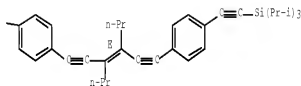
RN 864684-31-1 CAPLUS

CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-(4-[2-(tris(1-methylethyl)silyl]ethynyl)phenyl]-3-hexene-1,5-diyn-1-yl)phenyl]-4-[(3E)-3-propyl-4-[2-(4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-(4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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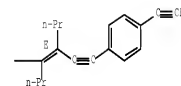
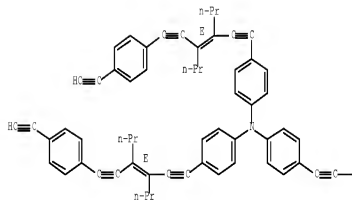


RN 864684-32-2 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-1-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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IT 740810-66-6P 740610-69-5P 864684-33-2P

864684-35-4P 864684-07-3P 864684-11-3P

864684-22-0P 864684-23-1P 864684-24-2P

864684-25-3P 864684-26-4P 864684-27-5P

864684-28-6P 864684-29-7P 864684-30-8P

864684-33-3P

RL: DEV (Device component use); IMP (Industrial manufacture); SEN

(Synthetic preparation); TEM (Technical or engineered material use); PREP

(Preparation); USES (Uses)

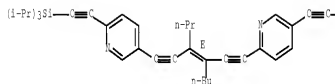
(preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic electrical component devices)

RN 740810-66-6 CAPLUS

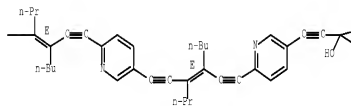
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

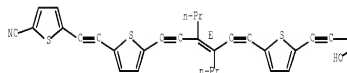
Double bond geometry as shown.

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PAGE 1-B

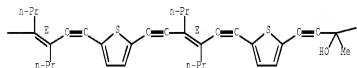
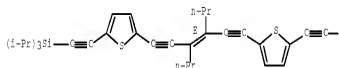




RN 740810-69-9 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-03-7 CAPLUS

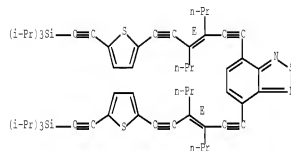
CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-[3-hydroxy-3-methyl-1-butyne-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

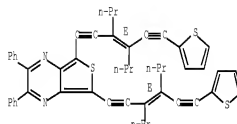
Double bond geometry as shown.



RN 864684-03-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-[2-thienyl]-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-[2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

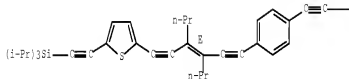


RN 864684-21-9 CAPLUS

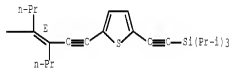
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-3-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B

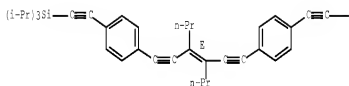


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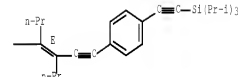
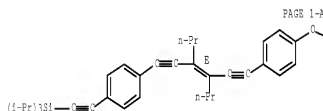
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B

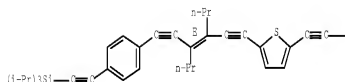


RN 864684-23-1 CAPLUS

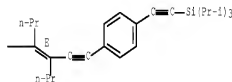
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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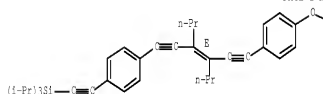


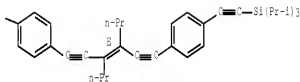
RN 864684-24-2 CAPLUS

CN Silane, [oxybis(4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl)]bis(tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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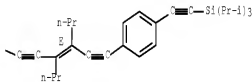
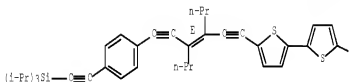




RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

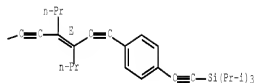
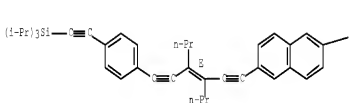
Double bond geometry as shown.



RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

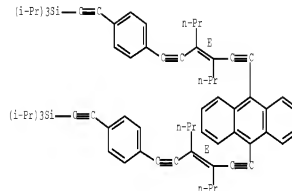
Double bond geometry as shown.



RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

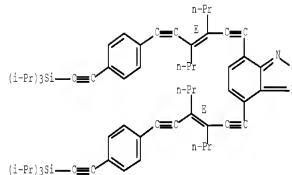
Double bond geometry as shown.



RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

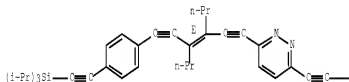


RN 864684-29-7 CAPLUS

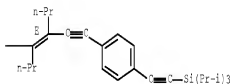
CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

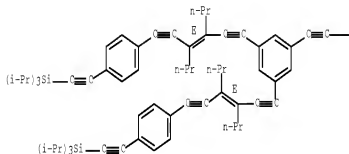


RN 864684-30-0 CAPLUS

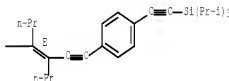
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

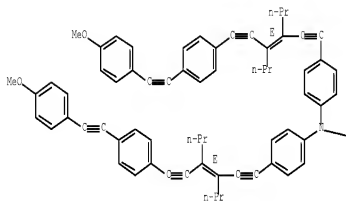


RN 864684-33-3 CAPLUS

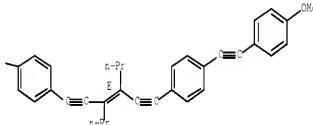
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

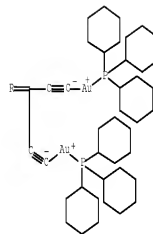


PAGE 1-B



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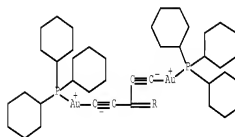
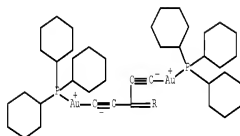
L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STM
 ACCESSION NUMBER: 2003:189466 CAPLUS Full-text
 DOCUMENT NUMBER: 139:101213
 TITLE: Luminescent properties of carbon-rich starburst gold(I) acetylide complexes. Crystal structure of [TEB][Au(PCy3)]4 ([TEB]H4 = tetraethynylethene)
 AUTHOR(S): Lu, Wei; Zhu, Xianrong; Che, Chi-Ming
 CORPORATE SOURCE: Department of Chemistry and HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Hong Kong, Peop. Rep. China
 SOURCE: Journal of Organometallic Chemistry (2003), 670 (1-2), 11-16
 CODEN: JORCAL; ISSN: 0022-328X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:101213
 AB Two carbon-rich starburst gold(I) acetylide complexes [TEB][Au(PCy3)]4 (3, [TEB]H4 = tetraethynylethene) and [TEB][Au(PCy3)]3 (6, [TEB]E3 = 1,3,5-triethynylbenzene) were prepared and their UV-vis absorption, emission and excitation spectra have been recorded. In fluid CH2Cl2 solns., 3 exhibits prompt 1($\pi\pi^*$) fluorescence with λ_{0-0} and λ_{max} at 413 and 428 nm, resp., while 6 displays 3($\pi\pi^*$) phosphorescence with λ_{0-0} and λ_{max} at 446 and 479 nm, resp. The crystal structure of 3-CH2Cl2 has been determined
 IT 558460-17-5P
 RI: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)
 RN 558460-17-6 CAPLUS
 CN Gold, [N-(3,4-di(ethynyl- κ C2)-3-hexene-1,5-diynato(4-))- κ Cl, κ C6]]tetrakis(tricyclohexylphosphine)tetra-, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 558460-16-5
 CRI C62 H132 Au4 P4
 CCI CCS



CM 2
 CRN 75-03-2
 CRI C H2 Cl2

CI=CH2=CI

IT 558460-16-5P
 RI: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (mol. structure, luminescence; preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)
 RN 558460-16-5 CAPLUS
 CN Gold, [N-(3,4-di(ethynyl- κ C2)-3-hexene-1,5-diynato(4-))- κ Cl, κ C6]]tetrakis(tricyclohexylphosphine)tetra- (9CI) (CA INDEX NAME)



RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)

CN Silane, 1,1'-[3,4-bis[2-(trimethylsilyl)ethynyl]-3-hexene-2,5-diyne-1,6-diyl]bis[1,1,1-trimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 30 THERE ARE 30 CAPLUS RECORDS THAT CITE THIS
RECORD (30 CITINGS)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> 13 and (electroluminescence or electroluminescent or luminescent or (light emitting) or OLED or (non linear optics) or NLO)

26473 ELECTROLUMINESCENCE
30 ELECTROLUMINESCENCES
26478 ELECTROLUMINESCENCE
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCES)
5 ELECTROLUMINESCENSE
26479 ELECTROLUMINESCENCE
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCE)
90044 ELECTROLUMINESCENT
8 ELECTROLUMINESCENTS
90047 ELECTROLUMINESCENT
(ELECTROLUMINESCENT OR ELECTROLUMINESCENTS)
65004 LUMINESCENT
10 LUMINESCENTS
65010 LUMINESCENT
(LUMINESCENT OR LUMINESCENTS)

1334311 LIGHT
12618 LIGHTS
1338543 LIGHT
(LIGHT OR LIGHTS)
140113 EMITTING
219 EMITTINGS
140157 EMITTING
(EMITTING OR EMITTINGS)
76113 LIGHT EMITTING
(LIGHT(W)EMITTING)
7493 OLED
3722 OLEDS
9385 OLED
(OLED OR OLEDS)
1110208 NON
38 NONS
1110237 NON
(NON OR NONS)
710357 LINEAR
74 LINEARS
710397 LINEAR
(LINEAR OR LINEARS)
53122 OPTICS
311 NON LINEAR OPTICS
(NON (W)LINEAR(W)OPTICS)
7807 NLO
19 NLOS
7820 NLO
(NLO OR NLOS)

L5 6 L3 AND (ELECTROLUMINESCENCE OR ELECTROLUMINESCENT OR LUMINESCENT OR (LIGHT EMITTING) OR OLED OR (NON LINEAR OPTICS) OR NLO)

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=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y
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ANSWER 1 OF 6 CAPUS COPYRIGHT 2009 ACS ON STM
ACCESSION NUMBER: 20064837081 CAPUS Full-text
DOCUMENT NUMBER: 14710411
TITLE: Theoretical design of light-emitting polymers - substitution effects of excited state ordering of polydiacetylene and polyacetylene
AUTHOR(S): Chen, Liping; Hou, Xingjun; Zhu, Lingyun; Yin, Shiwai; Shuai, Z.
CORPORATE SOURCE: Key Laboratory of Organic Solids, Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100080, Peop. Rep. China
SOURCE: Journal of Theoretical & Computational Chemistry (2006), 5(Spec. Issue), 391-400
CODEN: JTCGAC; ISSN: 0219-6336
PUBLISHER: World Scientific Publishing Co. Pte. Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The excited states structure, essential in determining the light-emitting properties, in a correlated electron system behaves differently from the one-electron system. Previous investigations show that upon proper chemical substitution, the non-emissive polyacetylene (PA) can be designed to be strongly light-emitting materials. On the basis of the correlated quantum chemical calcs. within the HDO/EM-COCD approach, we systematically studied both the pristine and substituted polydiacetylene (PDA) about the low-lying

excited states orderings. PDA possesses high mobility, but it is non-emissive. We predict that it is impossible to cause PDA to be light-emitting. From these numerical results, we propose a simple and practical rule to design conjugated light-emitting polymers, which require only a MO calcul. instead of sophisticated correlated calcons. This rule is derived from phys. pictures of correlated electron model, and is found to be in agreement with the existing expts. for various substituted PA and poly(p-phenylenebutadiynylene) (PPPB).

II 32803-11-3, 4-Octene-2,6-diyne 937386-11-3,
4,8-Dodecadiene-2,6,10-triyne 937386-12-4,
4,8,12-Hexadecatriene-2,6,10,14-tetrayne 937386-13-5
937386-14-6 937386-15-7 937386-15-1
937386-20-4 937386-21-5 937386-22-6
937386-23-7 937386-24-4

RL: FRP (Properties)

(theor. design of light-emitting polymers -
substitution effects of excited state ordering of polydiacetylene and
polyacetylene)

RN 32803-85-3 CAPLUS
CN 4-Octene-2,6-diyne (CA INDEX NAME)



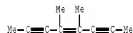
RN 937386-11-3 CAPLUS
CN 4,8-Dodecadiene-2,6,10-triyne (CA INDEX NAME)



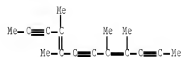
RN 937386-12-4 CAPLUS
CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne (CA INDEX NAME)



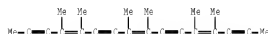
RN 937386-13-5 CAPLUS
CN 4-Octene-2,6-diyne, 4,5-dimethyl- (CA INDEX NAME)



RN 937386-14-6 CAPLUS
CN 4,8-Dodecadiene-2,6,10-triyne, 4,5,8,9-tetramethyl- (CA INDEX NAME)



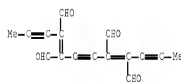
RN 937386-15-7 CAPLUS
CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne, 4,5,8,9,12,13-hexamethyl- (CA INDEX NAME)



RN 937386-19-1 CAPLUS
CN 2-Butenedial, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-20-4 CAPLUS
CN 2,6-Octadien-4-ynedicarboxaldehyde, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-21-5 CAPLUS
CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne-4,5,8,9,12,13-hexacarboxaldehyde (CA INDEX NAME)



RN 937386-22-6 CAPLUS
CN 2-Butenedinitrile, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)

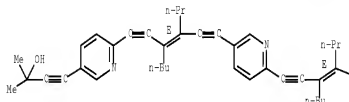


RN 740810-65-5 CAPLUS

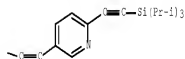
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-(tris[1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

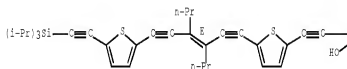


RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[[tris[1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

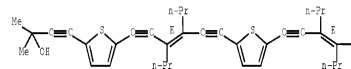


RN 740810-68-8 CAPLUS

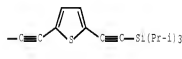
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[(3E)-3-propyl-4-[5-[[tris[1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



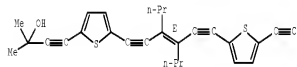
PAGE 1-B



RN 864683-96-5 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

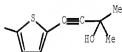
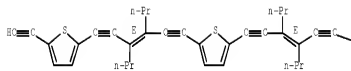
Double bond geometry as shown.



RN 864683-97-6 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-(5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

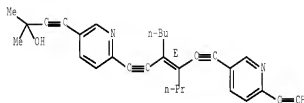
Double bond geometry as shown.



RN 864684-01-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

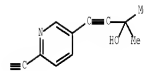
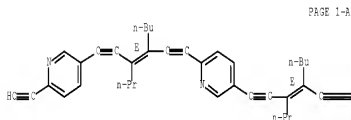
Double bond geometry as shown.



RN 864684-02-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

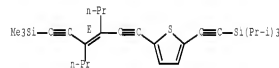
Double bond geometry as shown.



RN 864684-04-8 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

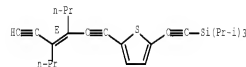
Double bond geometry as shown.



RN 864684-05-9 CAPLUS

CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

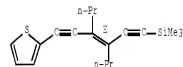
Double bond geometry as shown.



RN 864684-07-1 CAPLUS

CN Thiophene, 2-[(3E)-5-ethyl-3-propyl-4-[2-(trimethylsilyl)ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)

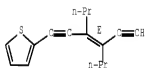
Double bond geometry as shown.



RN 864684-08-2 CAPLUS

CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



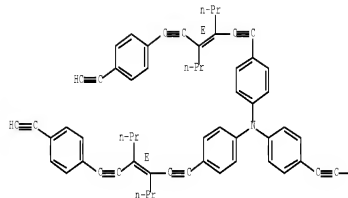
hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

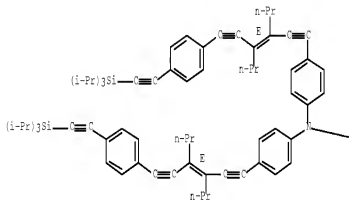
PAGE 1-A

RN 864684-31-1 CAPLUS
CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[2-(2-[tris(1-methylethyl)silyl]ethynyl]phenyl)-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-(4-[2-(tris(1-methylethyl)silyl]ethynyl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-(4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl)ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

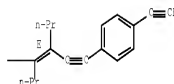


PAGE 1-A



PAGE 1-B

PAGE 1-B



IT 740810-66-6P 740810-67-3P 864684-03-7P
864684-06-0P 864684-09-3P 864684-21-9P
864684-27-0P 864684-28-1P 864684-24-2P
864684-25-3P 864684-26-4P 864684-23-5P
864684-28-6P 864684-29-7P 864684-30-3P
864684-33-0P

RI: DEV (Device component use); IMF (Industrial manufacture); SPW (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

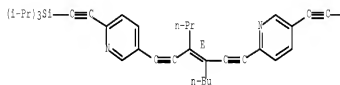
(preparation of π -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 864684-32-2 CAPLUS
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-

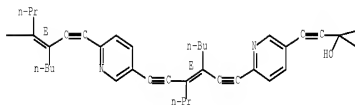
pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



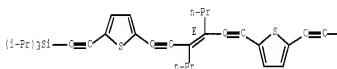
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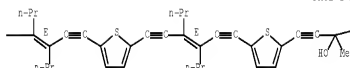
RN 740810-69-9 CAPLUS
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-(tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



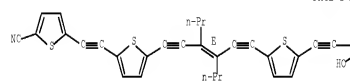
PAGE 1-C



RN 864684-03-7 CAPLUS
CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-[3-hydroxy-3-methyl-1-butyn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

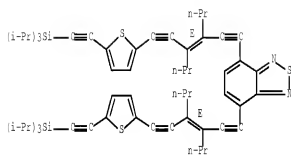


PAGE 1-B



RN 864684-06-0 CAPLUS
CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyne-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-(tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

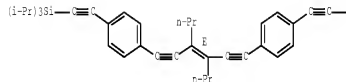
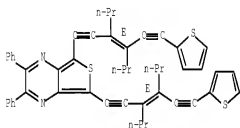
Double bond geometry as shown.

PAGE 1-A

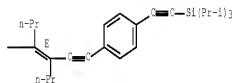
RN 864684-09-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-1-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

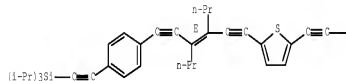
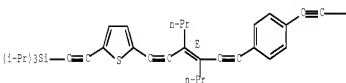
Double bond geometry as shown.

RN 864684-23-1 CAPLUS

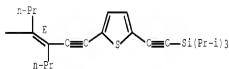
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

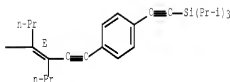
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



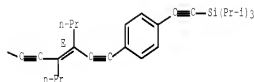


PAGE 1-B

RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

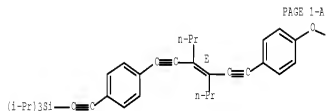


PAGE 1-B

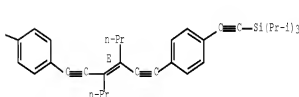
RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]-3-hexene-1,5-diyne-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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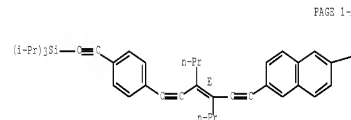


PAGE 1-B

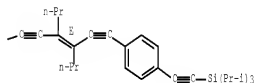
RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]-3-hexene-1,5-diyne-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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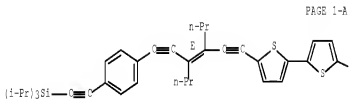


PAGE 1-B

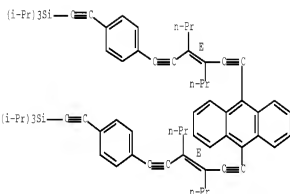
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]-3-hexene-1,5-diyne-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-(tris(1-methylethyl)silyl)ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



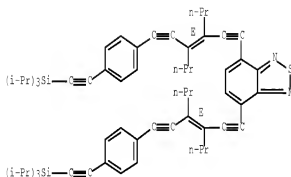
PAGE 1-A



RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

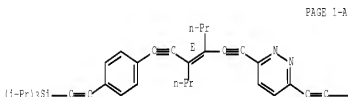
Double bond geometry as shown.



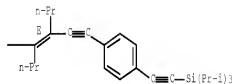
RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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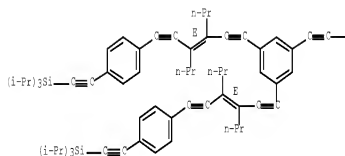


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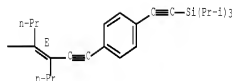
RN 864684-30-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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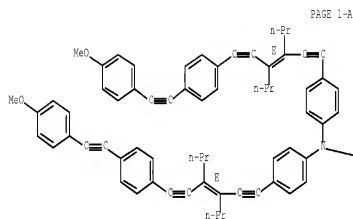


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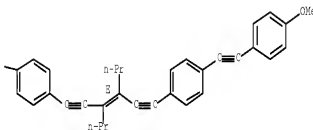
RN 864684-33-3 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-[4-methoxyphenyl]ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-[4-methoxyphenyl]ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-3-[4-[(3E)-4-[2-[4-[2-[4-methoxyphenyl]ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:73778 CAPLUS Full-text
 DOCUMENT NUMBER: 139:388935
 TITLE: Functional conjugated materials for optonics and electronics by tetraethynylethene molecular scaffolding
 AUTHOR(S): Nielsen, Moyens Brondsted; Diederich, Francois
 CORPORATE SOURCE: Laboratorium fuer Organische Chemie, HCI, ETH Hornggerberg, Zurich, CH-8093, Switz.
 SOURCE: Modern Arane Chemistry (2002), 196-216. Editor(s): Astruc, Didier. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany.
 CODEN: 69EMTX; ISSN: 3-527-30483-4
 DOCUMENT TYPE: Conference; General Review
 LANGUAGE: English
 AB A review; the phys. properties of scaffolds based on tetraethynylethene (TEE; 3,4-diethynylhex-3-ene-1,5-diyne) are strongly enhanced by arylation. Indeed, owing to the coplanarity of anilino-substituted TEE scaffolds, very high

third-order optical nonlinearities are obtained. Moreover, arylated TEEs are able to undergo photochem. induced cis-trans isomerization, paving the way for applications as light-driven mol. switches in optoelectronic devices. Suitably functionalized TEE modules are readily incorporated into linear and cyclic n-conjugated scaffolds, employing stepwise acetylenic coupling protocols. Thus, TEE mol. scaffolding has provided access to large, macrocyclic, all-carbon cores and long poly(triacetylene) (PTA) oligomers.

IT 133968-85-10, Tetraethynylethene, aryl. derivs.
 RI: DEV (Device component use); USES (Uses)
 (functional conjugated materials for optonics and electronics by tetraethynylethene mol. scaffolding)

RN 133968-85-1 CAPLUS
 CN 3-Hexene-1,5-diyne, 3,4-diethynyl- (CA INDEX NAME)

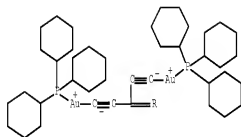


OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
 REFERENCE COUNT: 110 THERE ARE 110 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

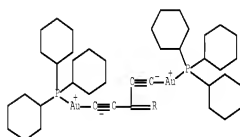
L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2003:189466 CAPLUS Full-text
 DOCUMENT NUMBER: 139:101213
 TITLE: Luminescent properties of carbon-rich starburst gold(I) acetylide complexes. Crystal structure of [TEE][Au(PCy3)]4 ((TEE)H4 = tetraethynylethene)
 AUTHOR(S): Lu, Wei; Zhu, Nanyong; Cha, Chi-Ming
 CORPORATE SOURCE: Department of Chemistry and HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Hong Kong, Peop. Rep. China
 SOURCE: Journal of Organometallic Chemistry (2003), 670(1-2), 11-16
 CODEN: JORCAJ; ISSN: 0022-328X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:101213
 AB Two carbon-rich starburst gold(I) acetylide complexes [TEE][Au(PCy3)]4 (3, [TEE]H4 = tetraethynylethene) and [TEE][Au(PCy3)]3 (6, [TEE]H3 = 1,3,5-triethynylbenzene) were prepared and their UV-vis absorption, emission and excitation spectra have been recorded. In fluid CH2Cl2 solns., 3 exhibits prompt 1(π*) fluorescence with λ0-0 and λmax at 413 and 428 nm, resp., while 6 displays 3(π*) phosphorescence with λ0-0 and λmax at 446 and 479 nm, resp. The crystal structure of 3-CH2Cl2 has been determined
 IT 559460-17-6P
 RI: PREP (Properties); SYN (Synthetic preparation); PREP (Preparation) (crystal structure); preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)
 RN 559460-17-6 CAPLUS
 CN Gold, [μ-(3,4-di(ethynyl)-xyl)-3-hexene-1,5-diyneato(4-)-]

CRN 558460-16-5
CMF C82 H132 Au4 P4
CCI CCS

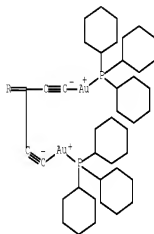
RU: PEP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (mol. structure, luminescence; preparation and luminescent
 properties of carbon-rich starburst gold acetylide complexes and
 crystal structure of tetraethynylethene gold phosphine complex)
 58460-16-5 CAPLUS
 Gold, [μ-(3,4-di(ethynyl)-κC2)-3-hexene-1,5-diyne(4-)-
 κC1,κC6)]tetrakis(tricyclohexylphosphine)tetra- (PCI) (CA
 INDEX NAME)



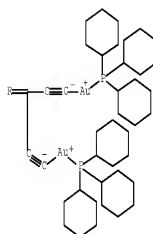
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CRN 75-09-2
CMF C H2 C12

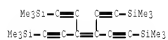
$$\text{Cl}-\text{CH}_2-\text{Cl}$$

IT 5560-75-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and luminescent properties of carbon-rich starburst
gold acetylide complexes and crystal structure of tetraethynylethene
gold phosphine complex)

RN 55660-76-9 CAPLUS

CN Silane, 1,1'-[3,4-bis[2-(trimethylsilyl)ethynyl]-3-hexene-2,5-diyne-1,6-diyl]bis[1,1,1-trimethyl- (CA INDEX NAME)



IT 558460-16-58

OS.CITING REF COUNT: 30 THERE ARE 30 CAPLUS RECORDS THAT CITE THIS RECORD (30 CITINGS)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:240433 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:19763

TITLE: Pt-tetraethynylethane molecular scaffolding: synthesis and characterization of a novel class of organometallic molecular rods

AUTHOR(S): Siemsen, Peter; Gubler, Ulrich; Bosshard, Christian; Gunter, Peter; Diederich, Francois

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, 8092, Switz.

SOURCE: Chemistry--A European Journal (2001), 7(6), 1333-1341

CODEN: CEUJED; ISSN: 0947-6539

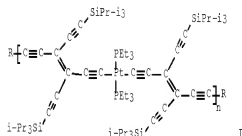
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:19763

GI



AB The series of monodisperse Pt-bridged TEE oligomers I (R = C.tpbond.CPH; n = 1-6) was prepared by oxidative Glaser - Hay oligomerization of monomer 7 under endcapping conditions. These novel mol. rods extend in length from 3.3 nm to 12.1 nm. Their isolation was achieved by high performance gel permeation chromatog. (GPC), and their purification was best monitored by anal. GPC in combination with matrix-assisted laser-desorption-ionization mass spectrometry (MALDI-TOF MS). The mass spectra of each oligomer revealed the mol. ion or its sodium complex as parent ion together with a clear, highly characteristic fragmentation pattern. Delayed addition of the end-capping reagent PhOCE to the oligomerization mixture afforded polymer I (R = B; n = 1) with an average of 432 repeat units and a remarkably narrow mol. weight distribution (Mw/Mn = 1.06), which is indicative of a living polymerization process. UV/Vis spectral data as well as measurements of the second hyperpolarizability $\chi^{(2)}$ by third harmonic generation (THG) revealed a nearly complete lack of π -electron delocalization along the oligomeric backbone. The Pt atoms act as true insulating centers, and the Pt-C(sp) bonds hardly possess any π character. The synthesis of the mol. rods I provides another demonstration of the power of oxidative acetylenic homocouplings for the preparation of unusual nanoarchitecture.

IT 155063-39-1

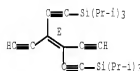
RL: RCT (Reactant); RACT (Reactant or reagent)

(Hagihara coupling of)

RN 155063-39-1 CAPLUS

CN Silane, 1,1'-[(3E)-3,4-diethynyl-3-hexene-1,5-diyne]-bis[1,1,1-tris(1-methylethyl)-] (CA INDEX NAME)

Double bond geometry as shown.



IT 177500-66-2

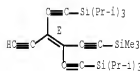
RL: RCT (Reactant); RACT (Reactant or reagent)

(Hagihara coupling of, to form corresponding platinum bis(acetylide) complex)

RN 177500-66-2 CAPLUS

CN Silane, [(3E)-3-ethynyl-4-[(trimethylsilyl)ethynyl]-3-hexene-1,5-diyne-1,6-diyl]bis[tris(1-methylethyl)-] (9CI) (CA INDEX NAME)

Double bond geometry as shown.



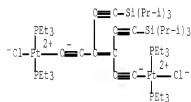
IT 342665-85-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(failed reaction; preparation and attempted oligomerization of)

RN 342665-85-2 CAPLUS

CN Platinum, [mu-[(3E)-3,4-bis[[(tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diyne-1,6-diyl]]dichlorotetrakis(triethylphosphine)di-, stereoisomer (9CI) (CA INDEX NAME)



IT 342993-88-5P

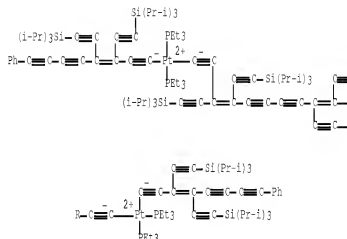
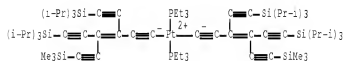
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and desilylation of)

RN 342885-88-5 CAPLUS

CN Platinum, bis(triethylphosphine)bis[(3Z)-6-(trimethylsilyl)-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diynyl]-, (SP-4-1)- (9CI) (CA INDEX NAME)

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IT 342885-89-116, terminated by phenylacetylene

342885-50-5E 342885-91-0U 342885-94-1P
RI: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and nonlinear optical properties of)

RN 342885-89-6 CAPLUS

CN Platinum, bis[(3Z)-4-ethynyl-6-(tris(1-methylethyl)silyl)-3-[[tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diynyl]bis(triethylphosphine)-, (SP-4-1)-, homopolymer (9CI) (CA INDEX NAME)

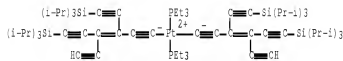
CM 1

PAGE 1-B

CRN 342885-86-3

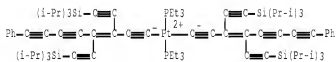
CNF C68 H116 P2 Pt Si4

CCI CCS



RN 342885-90-9 CAPLUS

CN Platinum, bis[(3Z)-8-phenyl-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-octene-1,5,7-triynyl]bis(triethylphosphine)-, (SP-4-1)- (9CI) (CA INDEX NAME)



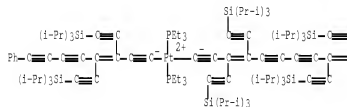
RN 342885-92-1 CAPLUS

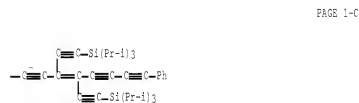
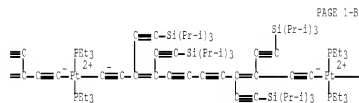
CN Platinum, bis[(3Z)-8-phenyl-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-octene-1,5,7-triynyl]bis[μ-[(3Z,9Z)-3,4,9,10-tetrakis[[tris(1-methylethyl)silyl]ethynyl]-3,9-dodecadiene-1,5,7,11-tetrayne-1,12-diyl]]hexakis(triethylphosphine)/tri-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

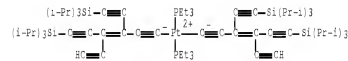
RN 342885-91-0 CAPLUS

CN Platinum, bis[(3Z)-8-phenyl-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-octene-1,5,7-triynyl][μ-[(3Z,9Z)-3,4,9,10-tetrakis[[tris(1-methylethyl)silyl]ethynyl]-3,9-dodecadiene-1,5,7,11-tetrayne-1,12-diyl]]tetrakis(triethylphosphine)/di-, stereoisomer (9CI) (CA INDEX NAME)





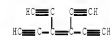
IT 342885-86-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and oxidative Glaser-Hay oligomerization of)
 RN 342885-86-3 CAPLUS
 CN Platinum, bis[(3,7)-4-ethynyl-6-(tris(1-methylethyl)silyl)-3-[(tris(1-methylethyl)silyl)ethynyl]-3-hexene-1,5-diynyl]bis(triethylphosphine)-, (SP-4-1)- (9CI) (CA INDEX NAME)



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L5 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS ON SIN
 ACCESSION NUMBER: 1999:370934 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 131:31961
 TITLE: Tetraethynylethenes: versatile carbon-rich building blocks for two-dimensional acetylenic scaffolding
 AUTHOR(S): Diederich, Francois
 CORPORATE SOURCE: Department of Chemistry, Swiss Federal Institute of Technology, Zurich, CH-8032, Switz.
 SOURCE: NATO ASI Series, Series C: Mathematical and Physical Sciences (1997), 499 (Modular Chemistry), 17-31
 CODEX: NSC50W; ISSN: 0258-2023
 PUBLISHER: Kluwer Academic Publishers
 DOCUMENT TYPE: Journal; General Review

LANGUAGE: English
 AB Derivs. of tetraethynylethene (TEE, 3,4-diethynyl-hex-3-ene-1,5-diyne) constitute a versatile mol. construction kit for acetylenic mol. scaffolding. TEEs were introduced into multianometer-sized functional mol. and polymeric materials with stable, extended C cores that exhibit unusual electronic and optical properties. The planar TEE C frame is a basic repeat unit for the construction of two-dimensional crystalline all-C networks. Starting from cis-bis-deprotected TEEs, annulenes were prepared as macrocyclic precursors to such networks. The challenges encountered in the formation of extended regular C networks by oxidative acetylenic coupling are discussed, and techniques from supramol. chemical probably overcome the difficulties that prevented their preparation so far. One approach consists in the self-assembly of metal-acetylenic networks under thermodyn. control and error checking, followed by reductive elimination of the metal centers to the all-C net. Expanded radialenes represent another class of stable, extended C-rich compds. which were prepared for the 1st time starting from TEE precursors. Trans-bis-deprotected TEEs provided access to rod-like oligomers and polymers with the novel polytriacyetylene (PTA) backbone. The redox-properties of these remarkably stable materials are discussed. Tetraakis(phenylethynyl)ethene forms highly ordered charge-transfer complexes with π -acceptors in the solid state and in solution. By attaching p-donor and p-acceptor substituted Ph rings to TEEs, novel M/O materials were obtained. It was shown for a large class of TEEs that donor/acceptor substitutions and fully two-dimensional conjugation strongly enhance the 3rd-order nonlinear optical properties. The relevance of the results obtained from studies of extended unsatd. C-rich materials for C allotropy in general is discussed. A review with 30 refs.
 IT 133968-85-1RG; Tetraethynylethene, organic derivs.
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (as versatile carbon-rich building blocks for two-dimensional acetylenic scaffolding)
 RN 133968-85-1 CAPLUS
 CN 3-Hexene-1,5-diyne, 3,4-diethynyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
 REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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